

## Chemical Safety Data Sheet MSDS / SDS

## Acetoacetanilide SDS

Revision Date:2024-04-25 Revision Number:1

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

Product name: Acetoacetanilide  
CAS: 102-01-2

**Relevant identified uses of the substance or mixture and uses advised against**

Relevant identified uses: For R&D use only. Not for medicinal, household or other use.  
Uses advised against: none

**Company Identification**

Company: Chemicalbook.in  
Address: 5 vasavi Layout Basaveswara Nilayam Pragathi Nagar Hyderabad, India -500090  
Telephone: +91 9550333722

**SECTION 2: Hazards identification****Classification of the substance or mixture**

Acute toxicity - Category 4, Oral  
Acute toxicity - Category 4, Dermal

Acute toxicity - Category 4, Inhalation  
Specific target organ toxicity - repeated exposure, Category 2

**GHS label elements, including precautionary statements**

Pictogram(s)



Signal word

Warning

**Hazard statement(s)**

H302+H312+H332 Harmful if swallowed, in contact with skin or if inhaled  
H373 May cause damage to organs through prolonged or repeated exposure

**Precautionary statement(s)**

**Prevention**

P264 Wash ... thoroughly after handling.  
P270 Do not eat, drink or smoke when using this product.  
P280 Wear protective gloves/protective clothing/eye protection/face protection/hearing protection/...  
P261 Avoid breathing dust/fume/gas/mist/vapours/spray.  
P271 Use only outdoors or in a well-ventilated area.  
P260 Do not breathe dust/fume/gas/mist/vapours/spray.

**Response**

P301+P317 IF SWALLOWED: Get medical help.  
P330 Rinse mouth.  
P302+P352 IF ON SKIN: Wash with plenty of water/...  
P317 Get medical help.  
P321 Specific treatment (see ... on this label).  
P362+P364 Take off contaminated clothing and wash it before reuse.  
P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.  
P319 Get medical help if you feel unwell.

**Storage**

none

**Disposal**

P501 Dispose of contents/container to an appropriate treatment and disposal facility in accordance with applicable laws and regulations, and product characteristics at time of disposal.

**Other hazards which do not result in classification**

no data available

**SECTION 3: Composition/information on ingredients**

**Substance**

Chemical name: Acetoacetanilide

Common names and synonyms: Acetoacetanilide

CAS number: 102-01-2

EC number: 202-996-4

Concentration: 100%

**SECTION 4: First aid measures**

**Description of necessary first-aid measures**

**If inhaled**

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately. Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

**Following skin contact**

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

**Following eye contact**

Rinse with pure water for at least 15 minutes. Consult a doctor.

**Following ingestion**

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

### **Most important symptoms/effects, acute and delayed**

ACUTE/CHRONIC HAZARDS: This compound is a weak allergen. When heated to decomposition it emits toxic fumes. (NTP, 1992)

### **Indication of immediate medical attention and special treatment needed, if necessary**

no data available

## **SECTION 5: Firefighting measures**

### **Suitable extinguishing media**

Alcohol foam, water mist, carbon dioxide, dry chemical.

### **Specific hazards arising from the chemical**

This chemical is combustible. (NTP, 1992)

### **Special protective actions for fire-fighters**

Wear self-contained breathing apparatus for firefighting if necessary.

## **SECTION 6: Accidental release measures**

### **Personal precautions, protective equipment and emergency procedures**

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

### **Environmental precautions**

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

### **Methods and materials for containment and cleaning up**

Collect and arrange disposal. Keep the chemical in suitable and closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Adhered or collected material should be promptly disposed of, in accordance

with appropriate laws and regulations.

## **SECTION 7: Handling and storage**

### **Precautions for safe handling**

Handling in a well ventilated place. Wear suitable protective clothing. Avoid contact with skin and eyes. Avoid formation of dust and aerosols. Use non-sparking tools. Prevent fire caused by electrostatic discharge steam.

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

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

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

### **Control parameters**

#### **Occupational Exposure limit values**

no data available

#### **Biological limit values**

no data available

### **Appropriate engineering controls**

Ensure adequate ventilation. Handle in accordance with good industrial hygiene and safety practice. Set up emergency exits and the risk-elimination area.

### **Individual protection measures, such as personal protective equipment (PPE)**

#### **Eye/face protection**

Wear tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

#### **Skin protection**

Wear fire/flame resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived

from it.

### Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

### Thermal hazards

no data available

## SECTION 9: Physical and chemical properties and safety characteristics

Physical state:	Solid. Powder.
Colour:	White.
Odour:	no data available
Melting point/freezing point:	78 °C. Atm. press.:1 013 hPa.
Boiling point or initial boiling point and boiling range:	181°C
Flammability:	no data available
Lower and upper explosion limit/flammability limit:	no data available
Flash point:	160°C(lit.)
Auto-ignition temperature:	> 440 °C.
Decomposition temperature:	no data available
pH:	no data available
Kinematic viscosity:	no data available
Solubility:	less than 1 mg/mL at 70° F (NTP, 1992)

Partition coefficient n-octanol/water:	log Pow = 0.93. Temperature:23 °C.
Vapour pressure:	Ca. 0.013 Pa. Temperature:Ca. 50 °C.;Ca. 0 Pa. Temperature:Ca. 25 °C.;Ca. 0 Pa. Temperature:Ca. 20 °C.
Density and/or relative density:	Ca. 0.45 g/cm <sup>3</sup> . Temperature:24 °C.
Relative vapour density:	6.1 (vs air)
Particle characteristics:	no data available

## SECTION 10: Stability and reactivity

### Reactivity

no data available

### Chemical stability

Enol form is unstable

### Possibility of hazardous reactions

**FIRE HAZARD: SLIGHT, WHEN EXPOSED TO HEAT OR FLAME.** Organic amides react with azo and diazo compounds to generate toxic gases. Flammable gases are formed by the reaction of organic amides with strong reducing agents. Amides are very weak bases (weaker than water). Mixing amides with dehydrating agents such as P<sub>2</sub>O<sub>5</sub> or SOCl<sub>2</sub> generates the corresponding nitrile. The combustion of these compounds generates mixed oxides of nitrogen (NO<sub>x</sub>). Ketones are reactive with many acids and bases liberating heat and flammable gases (e.g., H<sub>2</sub>). The amount of heat may be sufficient to start a fire in the unreacted portion of the ketone. Ketones react with reducing agents such as hydrides, alkali metals, and nitrides to produce flammable gas (H<sub>2</sub>) and heat. Ketones are incompatible with isocyanates, aldehydes, cyanides, peroxides, and anhydrides. They react violently with aldehydes, HNO<sub>3</sub>, HNO<sub>3</sub> + H<sub>2</sub>O<sub>2</sub>, and HClO<sub>4</sub>.

### Conditions to avoid

no data available

**Incompatible materials**

See aniline. ...can react vigorously with oxidizing materials. aniline

**Hazardous decomposition products**

See aniline. ...when heated to decomp, it emits highly toxic fumes. aniline

**SECTION 11: Toxicological information****Acute toxicity**

Oral: LD50 - rat (female) - 5.4 g/kg bw.

Inhalation: no data available

Dermal: no data available

**Skin corrosion/irritation**

no data available

**Serious eye damage/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



**STOT-single exposure**

no data available

**STOT-repeated exposure**

no data available

**Aspiration hazard**

no data available

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

Toxicity to fish: LC50 - Danio rerio (previous name: Brachydanio rerio) - > 242 - < 332 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC10 - Daphnia magna - 12 mg/L - 24 h.

Toxicity to algae: EC50 - Pseudokirchneriella subcapitata (previous names: Raphidocelis subcapitata, Selenastrum capricornutum) - 318 mg/L - 72 h.

Toxicity to microorganisms: EC50 - activated sludge, industrial - 9 375 mg/L - 3 h. Remarks: Respiration rate.

**Persistence and degradability**

Biodegradation studies of acetoacetanilide based on COD measurements, using an activated sludge seed indicate that acetoacetanilide is biodegradable(1,2). One study used an initial concentration of acetoacetanilide of 248 ppm and reported an 18 percent COD removal over a period of 24 hours(1). A second study used an initial concentration of 100 ppm acetoacetanilide and reported an 87 percent COD removal over a 24 hour period(2).

**Bioaccumulative potential**

An estimated BCF value of 3.4 was calculated for acetoacetanilide(SRC), using an estimated log Kow of 1.0(1,SRC) and a recommended regression-derived equation(2). According to a classification scheme(3), this BCF value suggests that bioconcentration in aquatic organisms is low(SRC).

**Mobility in soil**

Using a structure estimation method based on molecular connectivity indices(1), the Koc for acetoacetanilide can be estimated to

be about 12(SRC). According to a recommended classification scheme(2), this estimated Koc value suggests that acetoacetanilide has very high mobility in soil(SRC).

#### **Other adverse effects**

no data available

### **SECTION 13: Disposal considerations**

#### **Disposal methods**

##### **Product**

The material can be disposed of by removal to a licensed chemical destruction plant or by controlled incineration with flue gas scrubbing. Do not contaminate water, foodstuffs, feed or seed by storage or disposal. Do not discharge to sewer systems.

##### **Contaminated packaging**

Containers can be triply rinsed (or equivalent) and offered for recycling or reconditioning. Alternatively, the packaging can be punctured to make it unusable for other purposes and then be disposed of in a sanitary landfill. Controlled incineration with flue gas scrubbing is possible for combustible packaging materials.

### **SECTION 14: Transport information**

#### **UN Number**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

#### **UN Proper Shipping Name**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

#### **Transport hazard class(es)**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

#### **Packing group, if applicable**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

#### **Environmental hazards**

ADR/RID: No

IMDG: No

IATA: No

#### **Special precautions for user**

no data available

#### **Transport in bulk according to IMO instruments**

no data available

### **SECTION 15: Regulatory information**

#### **Safety, health and environmental regulations specific for the product in question**

##### **European Inventory of Existing Commercial Chemical Substances (EINECS)**

Listed.

##### **EC Inventory**

Listed.

##### **United States Toxic Substances Control Act (TSCA) Inventory**

Listed.

##### **China Catalog of Hazardous chemicals 2015**

Not Listed.

### **New Zealand Inventory of Chemicals (NZIoC)**

Listed.

### **(PICCS)**

Listed.

### **Vietnam National Chemical Inventory**

Listed.

### **IECSC)**

Listed.

### **Korea Existing Chemicals List (KECL)**

Listed.

## **SECTION 16: Other information**

### **Abbreviations and acronyms**

CAS: Chemical Abstracts Service

ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road

RID: Regulation concerning the International Carriage of Dangerous Goods by Rail

IMDG: International Maritime Dangerous Goods

IATA: International Air Transportation Association

TWA: Time Weighted Average

STEL: Short term exposure limit

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

EC50: Effective Concentration 50%

### **References**

IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>

HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>

IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>

eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:  
[http://www.echemportal.org/echemportal/index?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)

CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>

ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>

ERG - Emergency Response Guidebook by U.S. Department of Transportation, website:  
<http://www.phmsa.dot.gov/hazmat/library/erg>

Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>

ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>

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