

ACETOACETANILIDE

GHS Safety Data Sheet

Version No:4

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Section 1 - CHEMICAL PRODUCT AND COMPANY IDENTIFICATION

PRODUCT NAME

ACETOACETANILIDE

OTHER NAMES

C10-H11-N-O2, C10-H11-N-O2, CH₃COCH₂CONHC₆H₅, AAN, "acetanilide, 2-acetyl-", "acetanilide, 2-acetyl-", acetoacetamidobenzene, "acetoacetic acid anilide", "acetoacetic anilide", ((acetoacetyl)amino)benzene, acetoacetylaniline, alpha-acetylacetanilide, N-(acetylacetyl)aniline, N-(acetylacetyl)aniline, "butanamide, 3-oxo-N-phenyl-", "butanamide, 3-oxo-N-phenyl-", beta-ketobutyranilide, 3-oxo-N-phenylbutanamide, 3-oxo-N-phenylbutanamide, N-phenylacetoacetamide, N-phenylacetoacetamide, "USAF EK-1239"

PRODUCT USE

Intermediate in the manufacture of dry colours generally referred to as Hansa and benzidine yellows. In rubber compounding.

SUPPLIER

Company: S D FINE - CHEM LIMITED

Address:

315- 317, T.V.IND.ESTATE,

248 WORLI ROAD,

MUMBAI- 400 030, INDIA

technical@sdfine.com

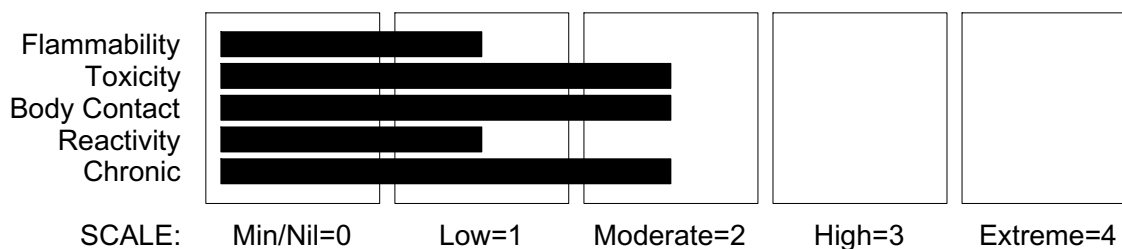
Telephone: 91- 22 24959898

Telephone: 91- 22 24959899

Fax: 91- 22 24937232

Section 2 - HAZARDS IDENTIFICATION

HAZARD RATINGS



GHS Classification

Acute Toxicity (Dermal) Category 4

Acute Toxicity (Oral) Category 4

Skin Sensitizer Category 1

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Section 2 - HAZARDS IDENTIFICATION



EMERGENCY OVERVIEW

HAZARD

WARNING

Determined by using GHS criteria:

H302 H312 H317

Harmful if swallowed

Harmful in contact with skin

May cause allergic skin reaction

PRECAUTIONARY STATEMENTS

Prevention

Avoid breathing dust/fume/gas/mist/vapours/spray.

Wash thoroughly after handling.

Do not eat, drink or smoke when using this product.

Contaminated work clothing should not be allowed out of the workplace.

Wear protective gloves/protective clothing/eye protection/face protection.

Response

IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell.

IF ON SKIN: Wash with plenty of soap and water.

Call a POISON CENTER or doctor/physician if you feel unwell.

Rinse mouth.

If skin irritation or rash occurs: Get medical advice/attention.

Wash contaminated clothing before reuse.

Section 3 - COMPOSITION / INFORMATION ON INGREDIENTS

NAME	CAS RN	%
acetoacetanilide	102-01-2	>98

Section 4 - FIRST AID MEASURES

SWALLOWED

- IF SWALLOWED, REFER FOR MEDICAL ATTENTION, WHERE POSSIBLE, WITHOUT DELAY.
- For advice, contact a Poisons Information Centre or a doctor.
- Urgent hospital treatment is likely to be needed.
- In the mean time, qualified first-aid personnel should treat the patient following observation and employing supportive measures as indicated by the patient's condition.
- If the services of a medical officer or medical doctor are readily available, the patient should be placed in his/her care and a copy of the MSDS should be provided. Further action will be the responsibility of the medical specialist.
- If medical attention is not available on the worksite or surroundings send the patient to a hospital

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Section 4 - FIRST AID MEASURES

together with a copy of the MSDS.

- Where medical attention is not immediately available or where the patient is more than 15 minutes from a hospital or unless instructed otherwise:
- INDUCE vomiting with fingers down the back of the throat, ONLY IF CONSCIOUS. Lean patient forward or place on left side (head-down position, if possible) to maintain open airway and prevent aspiration.

NOTE: Wear a protective glove when inducing vomiting by mechanical means.

EYE

- If this product comes in contact with the eyes:
- Wash out immediately with fresh running water.
- Ensure complete irrigation of the eye by keeping eyelids apart and away from eye and moving the eyelids by occasionally lifting the upper and lower lids.
- Seek medical attention without delay; if pain persists or recurs seek medical attention.
- Removal of contact lenses after an eye injury should only be undertaken by skilled personnel.

SKIN

- If skin contact occurs:
- Immediately remove all contaminated clothing, including footwear.
- Flush skin and hair with running water (and soap if available).
- Seek medical attention in event of irritation.

INHALED

- If dust is inhaled, remove from contaminated area.
- Encourage patient to blow nose to ensure clear passage of breathing.
- If irritation or discomfort persists seek medical attention.

NOTES TO PHYSICIAN

- The material may induce methaemoglobinaemia following exposure.
- Initial attention should be directed at oxygen delivery and assisted ventilation if necessary. Hyperbaric oxygen has not demonstrated substantial benefits.
- Hypotension should respond to Trendelenburg's position and intravenous fluids; otherwise dopamine may be needed.
- Symptomatic patients with methaemoglobin levels over 30% should receive methylene blue. (Cyanosis, alone, is not an indication for treatment). The usual dose is 1-2 mg/kg of a 1% solution (10 mg/ml) IV over 50 minutes; repeat, using the same dose, if symptoms of hypoxia fail to subside within 1 hour.
- Thorough cleansing of the entire contaminated area of the body, including the scalp and nails, is of utmost importance. BIOLOGICAL EXPOSURE INDEX - BEI

These represent the determinants observed in specimens collected from a healthy worker exposed at the Exposure Standard (ES or TLV):

Determinant	Index	Sampling Time	Comment
1. Methaemoglobin in blood	1.5% of haemoglobin	During or end of shift	B, NS, SQ

B: Background levels occur in specimens collected from subjects NOT exposed

NS: Non-specific determinant; also observed after exposure to other materials

SQ: Semi-quantitative determinant - Interpretation may be ambiguous; should be used as a screening test or confirmatory test.

Section 5 - FIRE FIGHTING MEASURES

EXTINGUISHING MEDIA

- Water spray or fog.
- Foam.

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Section 5 - FIRE FIGHTING MEASURES

- Dry chemical powder.
- BCF (where regulations permit).
- Carbon dioxide.

FIRE FIGHTING

- Alert Fire Brigade and tell them location and nature of hazard.
- Wear breathing apparatus plus protective gloves.
- Prevent, by any means available, spillage from entering drains or water courses.
- Use water delivered as a fine spray to control fire and cool adjacent area.
- DO NOT approach containers suspected to be hot.
- Cool fire exposed containers with water spray from a protected location.
- If safe to do so, remove containers from path of fire.
- Equipment should be thoroughly decontaminated after use.

FIRE/EXPLOSION HAZARD

- Combustible solid which burns but propagates flame with difficulty; it is estimated that most organic dusts are combustible (circa 70%) - according to the circumstances under which the combustion process occurs, such materials may cause fires and / or dust explosions.
 - Avoid generating dust, particularly clouds of dust in a confined or unventilated space as dusts may form an explosive mixture with air, and any source of ignition, i.e. flame or spark, will cause fire or explosion. Dust clouds generated by the fine grinding of the solid are a particular hazard; accumulations of fine dust (420 micron or less) may burn rapidly and fiercely if ignited - particles exceeding this limit will generally not form flammable dust clouds.; once initiated, however, larger particles up to 1400 microns diameter will contribute to the propagation of an explosion.
 - In the same way as gases and vapours, dusts in the form of a cloud are only ignitable over a range of concentrations; in principle, the concepts of lower explosive limit (LEL) and upper explosive limit (UEL).are applicable to dust clouds but only the LEL is of practical use; - this is because of the inherent difficulty of achieving homogeneous dust clouds at high temperatures (for dusts the LEL is often called the "Minimum Explosible Concentration", MEC)
 - A dust explosion may release of large quantities of gaseous products; this in turn creates a subsequent pressure rise of explosive force capable of damaging plant and buildings and injuring people.
 - Usually the initial or primary explosion takes place in a confined space such as plant or machinery, and can be of sufficient force to damage or rupture the plant. If the shock wave from the primary explosion enters the surrounding area, it will disturb any settled dust layers, forming a second dust cloud, and often initiate a much larger secondary explosion. All large scale explosions have resulted from chain reactions of this type.
 - Dry dust can be charged electrostatically by turbulence, pneumatic transport, pouring, in exhaust ducts and during transport.
 - Build-up of electrostatic charge may be prevented by bonding and grounding.
 - Powder handling equipment such as dust collectors, dryers and mills may require additional protection measures such as explosion venting.
 - All movable parts coming in contact with this material should have a speed of less than 1-meter/sec
 - A sudden release of statically charged materials from storage or process equipment, particularly at elevated temperatures and/ or pressure, may result in ignition especially in the absence of an apparent ignition source
 - One important effect of the particulate nature of powders is that the surface area and surface structure (and often moisture content) can vary widely from sample to sample, depending of how the powder was manufactured and handled; this means that it is virtually impossible to use flammability data published in the literature for dusts (in contrast to that published for gases and vapours).
 - Autoignition temperatures are often quoted for dust clouds (minimum ignition temperature (MIT)) and dust layers (layer ignition temperature (LIT)); LIT generally falls as the thickness of the layer increases.
- Combustion products include: carbon monoxide (CO), carbon dioxide (CO₂), nitrogen oxides (NO_x), other pyrolysis products typical of burning organic material.
- May emit poisonous fumes.
- May emit corrosive fumes.

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Section 5 - FIRE FIGHTING MEASURES

FIRE INCOMPATIBILITY

- Avoid contamination with oxidising agents i.e. nitrates, oxidising acids, chlorine bleaches, pool chlorine etc. as ignition may result.

PERSONAL PROTECTION

Glasses:

Chemical goggles.

Respirator:

Particulate

Section 6 - ACCIDENTAL RELEASE MEASURES

MINOR SPILLS

- Remove all ignition sources.
- Clean up all spills immediately.
- Avoid contact with skin and eyes.
- Control personal contact by using protective equipment.
- Use dry clean up procedures and avoid generating dust.
- Place in a suitable, labelled container for waste disposal.

MAJOR SPILLS

- Moderate hazard.
- CAUTION: Advise personnel in area.
- Alert Emergency Services and tell them location and nature of hazard.
- Control personal contact by wearing protective clothing.
- Prevent, by any means available, spillage from entering drains or water courses.
- Recover product wherever possible.
- IF DRY: Use dry clean up procedures and avoid generating dust. Collect residues and place in sealed plastic bags or other containers for disposal. IF WET: Vacuum/shovel up and place in labelled containers for disposal.
- ALWAYS: Wash area down with large amounts of water and prevent runoff into drains.
- If contamination of drains or waterways occurs, advise Emergency Services.

Personal Protective Equipment advice is contained in Section 8 of the MSDS.

Section 7 - HANDLING AND STORAGE

PROCEDURE FOR HANDLING

- Avoid all personal contact, including inhalation.
- Wear protective clothing when risk of exposure occurs.
- Use in a well-ventilated area.
- Prevent concentration in hollows and sumps.
- DO NOT enter confined spaces until atmosphere has been checked.
- DO NOT allow material to contact humans, exposed food or food utensils.
- Avoid contact with incompatible materials.
- When handling, DO NOT eat, drink or smoke.
- Keep containers securely sealed when not in use.
- Avoid physical damage to containers.
- Always wash hands with soap and water after handling.
- Work clothes should be laundered separately. Launder contaminated clothing before re-use.
- Use good occupational work practice.
- Observe manufacturer's storing and handling recommendations.
- Atmosphere should be regularly checked against established exposure standards to ensure safe working conditions are maintained.

Empty containers may contain residual dust which has the potential to accumulate following settling. Such dusts may explode in the presence of an appropriate ignition source.

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Section 7 - HANDLING AND STORAGE

- Do NOT cut, drill, grind or weld such containers
- In addition ensure such activity is not performed near full, partially empty or empty containers without appropriate workplace safety authorisation or permit.

SUITABLE CONTAINER

- Polyethylene or polypropylene container.
- Check all containers are clearly labelled and free from leaks.

STORAGE INCOMPATIBILITY

- Many arylamines (aromatic amines such as aniline, N-ethylaniline, o-toluidine, xylidine etc. and their mixtures) are hypergolic (ignite spontaneously) with red fuming nitric acid. When the amines are dissolved in triethylamine, ignition occurs at -60 deg. C. or less.
- Various metal oxides and their salts may promote ignition of amine-red fuming nitric acid systems. Soluble materials such as copper(I) oxide, ammonium metavanadate are effective; insoluble materials such as copper(II) oxide, iron(II) oxide, potassium dichromate are also effective.
- Avoid oxidising agents, acids, acid chlorides, acid anhydrides, chloroformates.

STORAGE REQUIREMENTS

- Store in original containers.
- Keep containers securely sealed.
- Store in a cool, dry, well-ventilated area.
- Store away from incompatible materials and foodstuff containers.
- Protect containers against physical damage and check regularly for leaks.
- Observe manufacturer's storing and handling recommendations.

SAFE STORAGE WITH OTHER CLASSIFIED CHEMICALS



+: May be stored together

O: May be stored together with specific precautions

X: Must not be stored together

Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION

EXPOSURE CONTROLS

The following materials had no OELs on our records

- acetoacetanilide:

CAS:102- 01- 2

MATERIAL DATA

ACETOACETANILIDE:

■ It is the goal of the ACGIH (and other Agencies) to recommend TLVs (or their equivalent) for all substances for which there is evidence of health effects at airborne concentrations encountered in the workplace.

At this time no TLV has been established, even though this material may produce adverse health effects (as evidenced in animal experiments or clinical experience). Airborne concentrations must be maintained as low as is practically possible and occupational exposure must be kept to a minimum.

NOTE: The ACGIH occupational exposure standard for Particles Not Otherwise Specified (P.N.O.S) does NOT apply.

Exposure limits with "skin" notation indicate that vapour and liquid may be absorbed through intact skin.

Absorption by skin may readily exceed vapour inhalation exposure. Symptoms for skin absorption are the same as for inhalation. Contact with eyes and mucous membranes may also contribute to overall exposure and may also invalidate the exposure standard.

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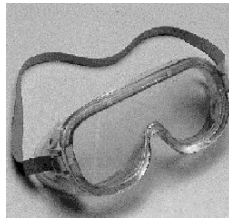
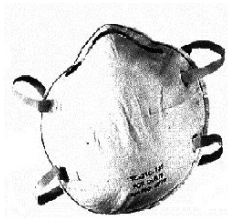
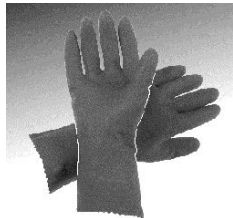
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Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION

OEL-STEL (Russia): 1 mg/m³ (skin)

PERSONAL PROTECTION



EYE

- Safety glasses with side shields.
- Chemical goggles.
- Contact lenses may pose a special hazard; soft contact lenses may absorb and concentrate irritants. A written policy document, describing the wearing of lens or restrictions on use, should be created for each workplace or task. This should include a review of lens absorption and adsorption for the class of chemicals in use and an account of injury experience. Medical and first-aid personnel should be trained in their removal and suitable equipment should be readily available. In the event of chemical exposure, begin eye irrigation immediately and remove contact lens as soon as practicable. Lens should be removed at the first signs of eye redness or irritation - lens should be removed in a clean environment only after workers have washed hands thoroughly. [CDC NIOSH Current Intelligence Bulletin 59].

HANDS/FEET

■ NOTE:

- The material may produce skin sensitisation in predisposed individuals. Care must be taken, when removing gloves and other protective equipment, to avoid all possible skin contact.
- Contaminated leather items, such as shoes, belts and watch-bands should be removed and destroyed. Suitability and durability of glove type is dependent on usage. Important factors in the selection of gloves include: such as:
 - frequency and duration of contact,
 - chemical resistance of glove material,
 - glove thickness and
 - dexterity

Select gloves tested to a relevant standard (e.g. Europe EN 374, US F739).

- When prolonged or frequently repeated contact may occur, a glove with a protection class of 5 or higher (breakthrough time greater than 240 minutes according to EN 374) is recommended.
- When only brief contact is expected, a glove with a protection class of 3 or higher (breakthrough time greater than 60 minutes according to EN 374) is recommended.
- Contaminated gloves should be replaced.

Gloves must only be worn on clean hands. After using gloves, hands should be washed and dried thoroughly. Application of a non-perfumed moisturiser is recommended.

Experience indicates that the following polymers are suitable as glove materials for protection against undissolved, dry solids, where abrasive particles are not present.

- polychloroprene
- nitrile rubber
- butyl rubber
- fluorocarbon
- polyvinyl chloride

Gloves should be examined for wear and/ or degradation constantly.

OTHER

- Overalls.
- P.V.C. apron.
- Barrier cream.
- Skin cleansing cream.

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Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION

- Eye wash unit.
- Respirators may be necessary when engineering and administrative controls do not adequately prevent exposures.
- The decision to use respiratory protection should be based on professional judgment that takes into account toxicity information, exposure measurement data, and frequency and likelihood of the worker's exposure - ensure users are not subject to high thermal loads which may result in heat stress or distress due to personal protective equipment (powered, positive flow, full face apparatus may be an option).
- Published occupational exposure limits, where they exist, will assist in determining the adequacy of the selected respiratory . These may be government mandated or vendor recommended.
- Certified respirators will be useful for protecting workers from inhalation of particulates when properly selected and fit tested as part of a complete respiratory protection program.
- Use approved positive flow mask if significant quantities of dust becomes airborne.
- Try to avoid creating dust conditions.

RESPIRATOR

Protection Factor	Half- Face Respirator	Full- Face Respirator	Powered Air Respirator
10 x ES	P1 Air- line*	- -	PAPR- P1 -
50 x ES	Air- line**	P2	PAPR- P2
100 x ES	-	P3	-
		Air- line*	-
100+ x ES	-	Air- line**	PAPR- P3

* - Negative pressure demand

** - Continuous flow.

The local concentration of material, quantity and conditions of use determine the type of personal protective equipment required. For further information consult your Occupational Health and Safety Advisor.

ENGINEERING CONTROLS

- Local exhaust ventilation is required where solids are handled as powders or crystals; even when particulates are relatively large, a certain proportion will be powdered by mutual friction.
- Exhaust ventilation should be designed to prevent accumulation and recirculation of particulates in the workplace.
- If in spite of local exhaust an adverse concentration of the substance in air could occur, respiratory protection should be considered. Such protection might consist of:
 - (a): particle dust respirators, if necessary, combined with an absorption cartridge;
 - (b): filter respirators with absorption cartridge or canister of the right type;
 - (c): fresh-air hoods or masks
- Build-up of electrostatic charge on the dust particle, may be prevented by bonding and grounding.
- Powder handling equipment such as dust collectors, dryers and mills may require additional protection measures such as explosion venting.

Air contaminants generated in the workplace possess varying "escape" velocities which, in turn, determine the "capture velocities" of fresh circulating air required to efficiently remove the contaminant.

Type of Contaminant:

direct spray, spray painting in shallow booths, drum filling, conveyer loading, crusher dusts, gas discharge (active generation into zone of rapid air motion)
grinding, abrasive blasting, tumbling, high speed wheel generated dusts (released at high initial velocity into zone of very high rapid air motion).

Air Speed:

1- 2.5 m/s (200- 500 f/min.)

2.5- 10 m/s (500- 2000 f/min.)

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Section 8 - EXPOSURE CONTROLS / PERSONAL PROTECTION

Within each range the appropriate value depends on:

Lower end of the range

- 1: Room air currents minimal or favourable to capture
- 2: Contaminants of low toxicity or of nuisance value only
- 3: Intermittent, low production.
- 4: Large hood or large air mass in motion

Upper end of the range

- 1: Disturbing room air currents
- 2: Contaminants of high toxicity
- 3: High production, heavy use
- 4: Small hood- local control only

Simple theory shows that air velocity falls rapidly with distance away from the opening of a simple extraction pipe. Velocity generally decreases with the square of distance from the extraction point (in simple cases). Therefore the air speed at the extraction point should be adjusted, accordingly, after reference to distance from the contaminating source. The air velocity at the extraction fan, for example, should be a minimum of 4-10 m/s (800-2000 f/min) for extraction of crusher dusts generated from the extraction point. Other mechanical considerations, producing performance deficits within the extraction apparatus, make it essential that theoretical air velocities are multiplied by factors of 10 or more when extraction systems are installed or used.

Section 9 - PHYSICAL AND CHEMICAL PROPERTIES

APPEARANCE

White, crystalline powder; mixes with water (8375-10000 mg/l). Soluble in dilute sodium hydroxide, alcohol, ether, acids, chloroform. The keto form (unlike the enol form) is stable.

PHYSICAL PROPERTIES

Solid.
Mixes with water.

State	Divided solid	Molecular Weight	177.20
Melting Range (°C)	85- 86	Viscosity	Not Applicable
Boiling Range (°C)	Not available	Solubility in water (g/L)	Miscible
Flash Point (°C)	162.7	pH (1% solution)	Not Available
Decomposition Temp (°C)	Not available.	pH (as supplied)	Not applicable
Autoignition Temp (°C)	450.56	Vapour Pressure (kPa)	Negligible
Upper Explosive Limit (%)	Not available.	Specific Gravity (water=1)	Not available
Lower Explosive Limit (%)	Not available	Relative Vapour Density (air=1)	6.1
Volatile Component (%vol)	Negligible	Evaporation Rate	Not applicable

Section 10 - CHEMICAL STABILITY AND REACTIVITY INFORMATION

CONDITIONS CONTRIBUTING TO INSTABILITY

- Presence of incompatible materials.
- Product is considered stable.
- Hazardous polymerisation will not occur.

For incompatible materials - refer to Section 7 - Handling and Storage.

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Section 11 - TOXICOLOGICAL INFORMATION

POTENTIAL HEALTH EFFECTS

ACUTE HEALTH EFFECTS

SWALLOWED

- Accidental ingestion of the material may be harmful; animal experiments indicate that ingestion of less than 150 gram may be fatal or may produce serious damage to the health of the individual.
- The substance and/or its metabolites may bind to haemoglobin inhibiting normal uptake of oxygen. This condition, known as "methaemoglobinemia", is a form of oxygen starvation (anoxia). Symptoms include cyanosis (a bluish discolouration skin and mucous membranes) and breathing difficulties. Symptoms may not be evident until several hours after exposure.

At about 15% concentration of blood methaemoglobin there is observable cyanosis of the lips, nose and earlobes. Symptoms may be absent although euphoria, flushed face and headache are commonly experienced. At 25-40%, cyanosis is marked but little disability occurs other than that produced on physical exertion. At 40-60%, symptoms include weakness, dizziness, lightheadedness, increasingly severe headache, ataxia, rapid shallow respiration, drowsiness, nausea, vomiting, confusion, lethargy and stupor. Above 60% symptoms include dyspnea, respiratory depression, tachycardia or bradycardia, and convulsions. Levels exceeding 70% may be fatal.

EYE

- Although the material is not thought to be an irritant (as classified by EC Directives), direct contact with the eye may cause transient discomfort characterised by tearing or conjunctival redness (as with windburn). Slight abrasive damage may also result. The material may produce foreign body irritation in certain individuals.

SKIN

- Skin contact with the material may be harmful; systemic effects may result following absorption.
- The material is not thought to be a skin irritant (as classified by EC Directives using animal models). Abrasive damage however, may result from prolonged exposures. Good hygiene practice requires that exposure be kept to a minimum and that suitable gloves be used in an occupational setting.
- Open cuts, abraded or irritated skin should not be exposed to this material.
- Entry into the blood-stream, through, for example, cuts, abrasions or lesions, may produce systemic injury with harmful effects. Examine the skin prior to the use of the material and ensure that any external damage is suitably protected.

INHALED

- The material is not thought to produce either adverse health effects or irritation of the respiratory tract following inhalation (as classified by EC Directives using animal models). Nevertheless, adverse systemic effects have been produced following exposure of animals by at least one other route and good hygiene practice requires that exposure be kept to a minimum and that suitable control measures be used in an occupational setting.
- Persons with impaired respiratory function, airway diseases and conditions such as emphysema or chronic bronchitis, may incur further disability if excessive concentrations of particulate are inhaled.

If prior damage to the circulatory or nervous systems has occurred or if kidney damage has been sustained, proper screenings should be conducted on individuals who may be exposed to further risk if handling and use of the material result in excessive exposures.

CHRONIC HEALTH EFFECTS

- Skin contact with the material is more likely to cause a sensitisation reaction in some persons compared to the general population.

Substance accumulation, in the human body, may occur and may cause some concern following repeated or long-term occupational exposure.

Long term exposure to high dust concentrations may cause changes in lung function i.e. pneumoconiosis; caused by particles less than 0.5 micron penetrating and remaining in the lung. Prime symptom is breathlessness; lung shadows show on X-ray.

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Section 11 - TOXICOLOGICAL INFORMATION

Most arylamines are powerful poisons to the blood-making system. High chronic doses cause congestion of the spleen and tumour formation.

TOXICITY AND IRRITATION

■ unless otherwise specified data extracted from RTECS - Register of Toxic Effects of Chemical Substances.

TOXICITY

Oral (rat) LD50: 4650 mg/kg

Oral (rat) LD50: 1131 mg/kg * * [Sigma/Aldrich]

Subcutaneous (rat) LD50: 7000 mg/kg

Oral (mouse) LD50: 3400 mg/kg

Intraperitoneal (mouse) LD50: 300 mg/kg

Oral (rabbit) LD50: 3925 mg/kg

Dermal (g.pig) LD50: >1000 mg/kg *

■ Contact allergies quickly manifest themselves as contact eczema, more rarely as urticaria or Quincke's oedema. The pathogenesis of contact eczema involves a cell-mediated (T lymphocytes) immune reaction of the delayed type. Other allergic skin reactions, e.g. contact urticaria, involve antibody-mediated immune reactions. The significance of the contact allergen is not simply determined by its sensitisation potential: the distribution of the substance and the opportunities for contact with it are equally important. A weakly sensitising substance which is widely distributed can be a more important allergen than one with stronger sensitising potential with which few individuals come into contact. From a clinical point of view, substances are noteworthy if they produce an allergic test reaction in more than 1% of the persons tested.

For acetoacetanilide (AAA)

Acute toxicity: There are several studies on experimental animals. Depending on the vehicle used, oral LD50 values for rats range from greater than 800 to 6500 mg/kg. In tests in which propylene glycol was the vehicle, the LD50 values were >5000 mg/kg. In tests in which starch (2%) or guar gum (0.5%) was used, the LD50 values were between 800 and 3200 mg/kg. In one dermal test, application of 1000 mg/kg of AAA to the skin of guinea pigs for 24 hr resulted in no systemic toxicity. Another study resulted in deaths of guinea pigs at the highest dose of 1000 mg/kg, resulting in an LD50 between 500 and 1000 mg/kg

AAA caused little or no irritation to the skin of rabbits exposed for 4 hours or to the skin of guinea pigs exposed for 24 hours

Ocular irritation in the rabbit is characterized as moderate; irritation of the conjunctiva occurred immediately after exposure but abated to slight or minimal within 24 hours. Irrigation of the eye immediately after exposure reduced the severity of the reaction. AAA was not found to be a dermal sensitizer

Repeat dose toxicity: Repeated oral exposure of rats to dose levels of >30 mg/kg/day may result in methaemoglobinaemia.. Rats treated with 0.1 or 1.0 % AAA in the diet (102.4 and 1001.7 mg/kg bw) for 14 days had signs of cyanosis at the high-dose, but no signs of toxicity were observed at the low -dose. The NOEL was 102.4 mg/kg/d.

Animals treated with 12, 100, or 850 mg/kg AAA by gavage for 28 days demonstrated evidence of systemic toxicity and neurotoxicity. Dose-dependent changes in haematology and serum chemistry occurred that were indicative of haemolytic anemia and methaemoglobinaemia, and these were statistically significant in the high and mid -dose groups. Compensatory erythropoiesis was confirmed in the evaluation of bone marrow smears. By the end of the 14-day recovery period, haematologic parameters were near normal with no evidence of anemia or methaemoglobinaemia.

Reproductive and Developmental Toxicity: The reproductive and developmental toxicities of AAA were evaluated in an OECD Reproductive/Developmental Toxicity Screening Study (TG 421). Dose levels of 3, 30, and 100 mg/kg were used with the highest dose level expected to result in methaemoglobinaemia. Mating and fertility were unaffected by treatment, and there were no microscopic lesions in the sex organs. There were no effects on gestation, implantation, or viability, and no effects were observed in the pups. The NOEL for reproductive toxicity and developmental toxicity was 100 mg/kg. There is no reproductive or developmental health hazard from exposure to AAA.

It is possible that the reversible haematotoxicity of AAA is a result of its metabolic conversion to aniline or a related metabolite. The EPA has suggested that aniline is the primary chemical of concern from AAA metabolism, and the Agency has suggested that the toxicity of AAA parallels that of aniline. Both substances cause methaemoglobinaemia. Both substances were found not to be teratogenic at dose levels that result in maternal toxicity. The dissimilarity between AAA and aniline is the total dose necessary to cause effects. Aniline is considered by the US EPA to be highly acutely toxic, while AAA is only slightly acutely toxic. A single oral dose of 50 mg aniline/kg bw to dogs can result in methaemoglobinaemia. By contrast, rats that

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Section 11 - TOXICOLOGICAL INFORMATION

consumed feed with 0.1% AAA (100 mg/kg) for 14 days had no adverse effects, and repeated treatment with 30 mg/kg for 6-8 weeks resulted in only minimal methaemoglobinaemia (< 5%) which is not considered to be clinically important. Therefore, while the biological effect may be similar, it is not reasonable to assume that the hazard of AAA to human health is equivalent to that of aniline

Genotoxicity: AAA was found to be not mutagenic in Salmonella typhimurium strains TA-97, TA-98, TA-100, or TA-1535 when tested with or without metabolic activation . In addition, no mutations were observed in human lymphocytes when tested in vitro in a standard OECD 473 study both with and without metabolic activation . The genetic toxicity of AAA has not been tested in vivo; however, a micronucleus test may not be appropriate because background levels of bone marrow micronuclei may increase in animals dosed with AAA due to compensatory responses to the haematologic effects of AAA.

Carcinogenicity Long-term carcinogenicity studies have not been conducted with AAA.

Section 12 - ECOLOGICAL INFORMATION

Refer to data for ingredients, which follows:

ACETOACETANILIDE:

■ For acetoacetanilide (AAA):

Environmental fate:

AAA is soluble in water and its octanol-water partition coefficient is moderately low, which suggests that AAA preferentially partitions into water. These conclusions are supported by Level I Fugacity modeling which indicates that, following release to the environment, equilibrium partitioning of AAA will result in the following pattern of distribution:

In air 1.361%

In soil 0.234%

In water 97.291%

In biota 0.021%

In suspended solids 0.002%

In sediment 1.092%

Photodegradation: Acetoacetanilide does not absorb wavelengths of light above 290 nm and thus will not be susceptible to direct (uncatalysed) photodegradation.

The reaction of acetoacetanilide with hydroxide [OH.] will be the only significant process by which this material will be removed from the atmosphere. Atmospheric residence time is estimated to be 192 hours .

Stability in Water: AAA has a neutral pH in water, and does not readily hydrolyze. Only 3.5% decomposition occurred after 167.5 days

Biodegradation: In tests conducted with activated sludge, biodegradation rates of 85% in 5 days and 51.6% in 21 days (based on carbon dioxide evolution) have been reported . AAA is considered inherently biodegradable.

Although AAA is inherently biodegradable, high concentrations may inhibit microbial activity. In tests with activated sludge, an AAA concentration of 2000 mg/L inhibited glucose metabolism by 40%; however, lower concentrations of 20 and 200 mg/L had no adverse effects.

Bioaccumulation: The octanol/water partition coefficient is low (log Kow = 0.70), suggesting that AAA is not lipophilic and is not likely to bioaccumulate.

Ecotoxicity:

Fish LC50 (96 h): >100 mg/l

Daphnia EC50 (24 h): 70-200 mg/l

Daphnia EC50 996 h): >100 mg/l (OECD Guideline)

Algae EC50 (7 h): Selenastrum capricornutum 318 mg/l; NOEC 180 mg/l (OECD TG 201)

The acute toxicity of AAA has been evaluated in a number of aquatic species using standard test methods. The fathead minnow, Zebra fish, and several invertebrate species including Daphnia have been tested. Zebra fish were exposed to 177, 235, 242, or 332 mg/L for 96 hours with mortality occurring only at 332 mg/L . Signs of toxicity, including abnormal swimming behavior and tremors or convulsions were observed in fish exposed to 242 mg/L, and reduced activity was observed in fish exposed to the two lowest concentrations. The 96-hr LC50 for fathead minnows was reported to be greater than 100 mg/L

Other invertebrates have also been exposed to a concentration of 100 mg/L without evidence of adverse effects

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Section 12 - ECOLOGICAL INFORMATION

. In all cases, the EC50 or LC50 concentration was greater than 100 mg/L for a 96-hour exposure.

The majority of results suggest that AAA is of low toxicity to aquatic organisms and is of low concern for environmental effects to these species even though the expected distribution in the environment favors partitioning into water.

Although a chronic test in Daphnia is not available, there is no reason to expect that chronic effects of AAA would differ markedly from acute effects. AAA hydrolyses only very slowly to the more toxic compound aniline. Studies indicate that under abiotic conditions only 3.6% of AAA is hydrolysed to aniline after 167.5 days.

■ Aromatic amines (arylamines), particularly primary aromatic amines, covalently and irreversibly bind to humic substances present in most natural waters.

All metabolites with moieties of: anilines, benzidines and toluidines are of environmental concern. Anilines and benzidines are both acutely toxic and toxic depending on the specific aquatic species (except algae). Toluidines represent a similar concern, It has been speculated that aqueous solutions of aromatic amines can be oxidised by organic radicals, but there are no actual data on reaction rates. Based on a study of reaction rate data for these compounds an estimate of the half-life of aromatic amines in water is approximately 100 days, assuming a peroxy radical concentration of 10-10 mole/L in sunlit, oxygenated water.

■ DO NOT discharge into sewer or waterways.

Ecotoxicity

Ingredient	Persistence: Water/Soil	Persistence: Air	Bioaccumulation	Mobility
acetoacetanilide	LOW		LOW	HIGH

Section 13 - DISPOSAL CONSIDERATIONS

• Containers may still present a chemical hazard/ danger when empty.

• Return to supplier for reuse/ recycling if possible.

Otherwise:

• If container can not be cleaned sufficiently well to ensure that residuals do not remain or if the container cannot be used to store the same product, then puncture containers, to prevent re-use, and bury at an authorised landfill.

• Where possible retain label warnings and MSDS and observe all notices pertaining to the product.

Legislation addressing waste disposal requirements may differ by country, state and/ or territory. Each user must refer to laws operating in their area. In some areas, certain wastes must be tracked.

A Hierarchy of Controls seems to be common - the user should investigate:

• Reduction

• Reuse

• Recycling

• Disposal (if all else fails)

This material may be recycled if unused, or if it has not been contaminated so as to make it unsuitable for its intended use. Shelf life considerations should also be applied in making decisions of this type. Note that properties of a material may change in use, and recycling or reuse may not always be appropriate.

• DO NOT allow wash water from cleaning or process equipment to enter drains.

• It may be necessary to collect all wash water for treatment before disposal.

• In all cases disposal to sewer may be subject to local laws and regulations and these should be considered first.

• Where in doubt contact the responsible authority.

• Recycle wherever possible.

• Consult manufacturer for recycling options or consult local or regional waste management authority for disposal if no suitable treatment or disposal facility can be identified.

• Dispose of by: burial in a land-fill specifically licenced to accept chemical and / or pharmaceutical wastes or Incineration in a licenced apparatus (after admixture with suitable combustible material)

• Decontaminate empty containers. Observe all label safeguards until containers are cleaned and destroyed.

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Section 14 - TRANSPORTATION INFORMATION

HAZCHEM:

☐ None

NOT REGULATED FOR TRANSPORT OF DANGEROUS GOODS: UN, IATA, IMDG

Section 15 - REGULATORY INFORMATION

REGULATIONS

acetoacetanilide (CAS: 102-01-2) is found on the following regulatory lists;

"Australia Inventory of Chemical Substances (AICS)", "OECD Representative List of High Production Volume (HPV) Chemicals"

Section 16 - OTHER INFORMATION

■ Classification of the preparation and its individual components has drawn on official and authoritative sources as well as independent review by the Classification committee using available literature references.

■ The (M)SDS is a Hazard Communication tool and should be used to assist in the Risk Assessment. Many factors determine whether the reported Hazards are Risks in the workplace or other settings. Risks may be determined by reference to Exposures Scenarios. Scale of use, frequency of use and current or available engineering controls must be considered.

The above information is believed to be accurate and represent the best information currently available to us, but does not represent any warranty expressed or implied of the properties of the product. User should make their own investigation to determine the suitability of the information for their particular purpose.

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