



## SAFETY DATA SHEET

### 3-Methyl-1-(4-sulfophenyl)-2-pyrazolin-5-one

According to the REACH etc. (Amendment etc.) (EU Exit) Regulations 2020 No. 1577, as amended.

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

##### 1.1. Product identifier

|                       |   |
|-----------------------|---|
| Product name          | 3-Methyl-1-(4-sulfophenyl)-2-pyrazolin-5-one                        |
| Chemical name         | 4-(3-methyl-5-oxo-2-pyrazolin-1-yl)benzenesulphonic acid            |
| Synonyms; trade names | 4-(4,5-dihydro-3-methyl-5-oxo-1H-pyrazol-1-yl)-benzenesulfonic acid |
| CAS number            | 89-36-1   |
| EC number             | 201-901-3   |

##### 1.2. Relevant identified uses of the substance or mixture and uses advised against

|                      |  |
|----------------------|--|
| Identified uses      | Research and development.                                  |
| Uses advised against | Not suitable for human consumption or veterinary purposes. |

##### 1.3. Details of the supplier of the safety data sheet

|          |   |
|----------|---|
| Supplier | Molekula Ltd.<br>Lingfield Way,<br>Darlington,<br>DL1 4XX,<br>United Kingdom<br>+44 (0) 3302000333<br>info@molekula.com |
|----------|---|

##### 1.4. Emergency telephone number

+44 (0) 7769276927

#### SECTION 2: Hazards identification

##### 2.1. Classification of the substance or mixture

###### Classification (SI 2019 No. 720)

|                       |  |
|-----------------------|--|
| Physical hazards      | Not Classified                         |
| Health hazards        | Skin Corr. 1B - H314 Eye Dam. 1 - H318 |
| Environmental hazards | Aquatic Chronic 3 - H412               |

##### 2.2. Label elements

|           |           |
|-----------|-----------|
| EC number | 201-901-3 |
|-----------|-----------|

###### Hazard pictograms



|             |        |
|-------------|--------|
| Signal word | Danger |
|-------------|--------|

## 3-Methyl-1-(4-sulfohenyl)-2-pyrazolin-5-one

|                                 |  |
|---------------------------------|--|
| <b>Hazard statements</b>        | H314 Causes severe skin burns and eye damage.<br>H412 Harmful to aquatic life with long lasting effects.   |
| <b>Precautionary statements</b> | P260 Do not breathe dust.<br>P264 Wash contaminated skin thoroughly after handling.<br>P273 Avoid release to the environment.<br>P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.<br>P301+P330+P331 IF SWALLOWED: Rinse mouth. Do NOT induce vomiting.<br>P303+P361+P353 IF ON SKIN (or hair): Take off immediately all contaminated clothing. Rinse skin with water or shower.<br>P304+P340 IF INHALED: Remove person to fresh air and keep comfortable for breathing.<br>P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.<br>P310 Immediately call a POISON CENTER/ doctor.<br>P363 Wash contaminated clothing before reuse.<br>P405 Store locked up.<br>P501 Dispose of contents/ container in accordance with national regulations. |

### 2.3. Other hazards

This substance is not classified as PBT or vPvB according to current UK criteria.

## SECTION 3: Composition/information on ingredients

### 3.1. Substances

|                         |  |
|-------------------------|--|
| <b>Product name</b>     | 3-Methyl-1-(4-sulfohenyl)-2-pyrazolin-5-one              |
| <b>Chemical name</b>    | 4-(3-methyl-5-oxo-2-pyrazolin-1-yl)benzenesulphonic acid |
| <b>CAS number</b>       | 89-36-1  |
| <b>EC number</b>        | 201-901-3  |
| <b>Chemical formula</b> | C10H10N2O4S  |

## SECTION 4: First aid measures

### 4.1. Description of first aid measures

|                                   |   |
|-----------------------------------|---|
| <b>General information</b>        | Get medical attention if any discomfort continues. Show this Safety Data Sheet to the medical personnel. Chemical burns must be treated by a physician.   |
| <b>Inhalation</b>                 | Move affected person to fresh air and keep warm and at rest in a position comfortable for breathing. Maintain an open airway. Loosen tight clothing such as collar, tie or belt. Rinse nose and mouth with water. Never give anything by mouth to an unconscious person. Get medical attention if symptoms are severe or persist. |
| <b>Ingestion</b>                  | Rinse mouth thoroughly with water. Give a few small glasses of water or milk to drink. Stop if the affected person feels sick as vomiting may be dangerous. Get medical attention.  |
| <b>Skin contact</b>               | It is important to remove the substance from the skin immediately. Rinse immediately with plenty of water. Continue to rinse for at least 15 minutes and get medical attention. Chemical burns must be treated by a physician.  |
| <b>Eye contact</b>                | Rinse immediately with plenty of water. Do not rub eye. Remove any contact lenses and open eyelids wide apart. Continue to rinse for at least 15 minutes and get medical attention.   |
| <b>Protection of first aiders</b> | It may be dangerous for first aid personnel to carry out mouth-to-mouth resuscitation.  |

### 4.2. Most important symptoms and effects, both acute and delayed

|                            |   |
|----------------------------|---|
| <b>General information</b> | The severity of the symptoms described will vary dependent on the concentration and the length of exposure. |
|----------------------------|---|

### 3-Methyl-1-(4-sulphophenyl)-2-pyrazolin-5-one

|                     |   |
|---------------------|---|
| <b>Inhalation</b>   | A single exposure may cause the following adverse effects: Severe irritation of nose and throat. Symptoms following overexposure may include the following: Corrosive to the respiratory tract. |
| <b>Ingestion</b>    | May cause chemical burns in mouth, oesophagus and stomach. Symptoms following overexposure may include the following: Severe stomach pain. Nausea, vomiting.                                    |
| <b>Skin contact</b> | Causes severe burns. Symptoms following overexposure may include the following: Pain or irritation. Redness. Blistering may occur.  |
| <b>Eye contact</b>  | Causes serious eye damage. Symptoms following overexposure may include the following: Pain. Profuse watering of the eyes. Redness.  |

#### **4.3. Indication of any immediate medical attention and special treatment needed**

|                             |                        |
|-----------------------------|------------------------|
| <b>Notes for the doctor</b> | Treat symptomatically. |
|-----------------------------|------------------------|

### **SECTION 5: Firefighting measures**

#### **5.1. Extinguishing media**

|                                       |  |
|---------------------------------------|--|
| <b>Suitable extinguishing media</b>   | Extinguish with alcohol-resistant foam, carbon dioxide, dry powder or water fog. Use fire-extinguishing media suitable for the surrounding fire. |
| <b>Unsuitable extinguishing media</b> | Do not use water jet as an extinguisher, as this will spread the fire.   |

#### **5.2. Special hazards arising from the substance or mixture**

|                                      |  |
|--------------------------------------|--|
| <b>Specific hazards</b>              | Severe corrosive hazard. Water used for fire extinguishing, which has been in contact with the product, may be corrosive.  |
| <b>Hazardous combustion products</b> | Thermal decomposition or combustion products may include the following substances: Very toxic or corrosive gases or vapours. Carbon monoxide (CO). Carbon dioxide (CO <sub>2</sub> ). Nitrous gases (NO <sub>x</sub> ). Sulphurous gases (SO <sub>x</sub> ). |

#### **5.3. Advice for firefighters**

|  |  |
|--|--|
| <b>Protective actions during firefighting</b>        | Avoid breathing fire gases or vapours. Evacuate area. Keep upwind to avoid inhalation of gases, vapours, fumes and smoke. Cool containers exposed to heat with water spray and remove them from the fire area if it can be done without risk. Cool containers exposed to flames with water until well after the fire is out. Avoid discharge to the aquatic environment. Control run-off water by containing and keeping it out of sewers and watercourses. If risk of water pollution occurs, notify appropriate authorities. |
| <b>Special protective equipment for firefighters</b> | Regular protection may not be safe. Wear chemical protective suit. Wear positive-pressure self-contained breathing apparatus (SCBA) and appropriate protective clothing. Firefighter's clothing will provide a basic level of protection for chemical incidents.   |

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

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

|                             |   |
|-----------------------------|---|
| <b>Personal precautions</b> | Wear protective clothing as described in Section 8 of this safety data sheet. No action shall be taken without appropriate training or involving any personal risk. Do not touch or walk into spilled material. Avoid inhalation of dust. Use suitable respiratory protection if ventilation is inadequate. Avoid contact with skin and eyes. |
|-----------------------------|---|

#### **6.2. Environmental precautions**

|                                  |   |
|----------------------------------|---|
| <b>Environmental precautions</b> | Avoid discharge into drains or watercourses or onto the ground. Avoid discharge to the aquatic environment. |
|----------------------------------|---|

#### **6.3. Methods and material for containment and cleaning up**

### 3-Methyl-1-(4-sulfohenyl)-2-pyrazolin-5-one

#### Methods for cleaning up

Wear protective clothing as described in Section 8 of this safety data sheet. Clear up spills immediately and dispose of waste safely. This product is corrosive. Collect spillage with a shovel and broom, or similar and reuse, if possible. Collect and place in suitable waste disposal containers and seal securely. Flush contaminated area with plenty of water. Wash thoroughly after dealing with a spillage. Dangerous for the environment. Do not empty into drains. For waste disposal, see Section 13.

#### 6.4. Reference to other sections

**Reference to other sections** For personal protection, see Section 8. See Section 11 for additional information on health hazards. See Section 12 for additional information on ecological hazards. For waste disposal, see Section 13.

## SECTION 7: Handling and storage

### 7.1. Precautions for safe handling

#### Usage precautions

Read and follow manufacturer's recommendations. Wear protective clothing as described in Section 8 of this safety data sheet. Keep away from food, drink and animal feeding stuffs. Keep container tightly sealed when not in use. This product is corrosive. Immediate first aid is imperative. Avoid discharge to the aquatic environment. Do not handle until all safety precautions have been read and understood. Do not handle broken packages without protective equipment. Do not reuse empty containers.

#### Advice on general occupational hygiene

Wash promptly if skin becomes contaminated. Take off contaminated clothing. Wash contaminated clothing before reuse.

### 7.2. Conditions for safe storage, including any incompatibilities

#### Storage precautions

Store away from incompatible materials (see Section 10). Store locked up. Keep only in the original container. Keep container tightly closed, in a cool, well ventilated place. Keep containers upright. Protect containers from damage.

Moisture sensitive. Store under inert gas.

#### Storage class

Non-combustible corrosive hazardous substances

### 7.3. Specific end use(s)

#### Specific end use(s)

The identified uses for this product are detailed in Section 1.2.

## SECTION 8: Exposure controls/Personal protection

### 8.1. Control parameters

### 8.2. Exposure controls

#### Protective equipment



#### Appropriate engineering controls

Provide adequate ventilation. Observe any occupational exposure limits for the product or ingredients.

#### Eye/face protection

Wear tight-fitting, chemical splash goggles or face shield. If inhalation hazards exist, a full-face respirator may be required instead.

### 3-Methyl-1-(4-sulfohenyl)-2-pyrazolin-5-one

|  |  |
|--|--|
| <b>Hand protection</b>                 | Wear protective gloves. The most suitable glove should be chosen in consultation with the glove supplier/manufacturer, who can provide information about the breakthrough time of the glove material. To protect hands from chemicals, wear gloves that are proven to be impervious to the chemical and resist degradation. Considering the data specified by the glove manufacturer, check during use that the gloves are retaining their protective properties and change them as soon as any deterioration is detected. Frequent changes are recommended. |
| <b>Other skin and body protection</b>  | Wear appropriate clothing to prevent any possibility of skin contact.  |
| <b>Hygiene measures</b>                | Wash after use and before eating, smoking and using the toilet. Do not eat, drink or smoke when using this product.  |
| <b>Respiratory protection</b>          | Ensure all respiratory protective equipment is suitable for its intended use and is 'UKCA'-marked. Check that the respirator fits tightly and the filter is changed regularly. Gas and combination filter cartridges suitable for intended use should be used. Full face mask respirators with replaceable filter cartridges suitable for intended use should be used. Half mask and quarter mask respirators with replaceable filter cartridges suitable for intended use should be used.   |
| <b>Environmental exposure controls</b> | Keep container tightly sealed when not in use. Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental protection legislation. In some cases, fume scrubbers, filters or engineering modifications to the process equipment will be necessary to reduce emissions to acceptable levels.  |

## SECTION 9: Physical and chemical properties

### 9.1. Information on basic physical and chemical properties

|   |                           |
|---|---------------------------|
| <b>Appearance</b>                                   | Solid.                    |
| <b>Colour</b>                                       | Off-white. Yellow. Red.   |
| <b>Odour</b>  | Not known.                |
| <b>Odour threshold</b>                              | No information available. |
| <b>pH</b>   | No information available. |
| <b>Melting point</b>                                | > 252°C/485.6°F           |
| <b>Initial boiling point and range</b>              | No information available. |
| <b>Flash point</b>                                  | No information available. |
| <b>Evaporation rate</b>                             | No information available. |
| <b>Flammability (solid, gas)</b>                    | No information available. |
| <b>Upper/lower flammability or explosive limits</b> | No information available. |
| <b>Vapour pressure</b>                              | No information available. |
| <b>Vapour density</b>                               | No information available. |
| <b>Relative density</b>                             | No information available. |
| <b>Solubility(ies)</b>                              | No information available. |
| <b>Partition coefficient</b>                        | No information available. |
| <b>Auto-ignition temperature</b>                    | No information available. |
| <b>Decomposition Temperature</b>                    | > 252°C/485.6°F           |

### 3-Methyl-1-(4-sulphophenyl)-2-pyrazolin-5-one

#### 9.2. Other information

Molecular weight 254.26

#### SECTION 10: Stability and reactivity

##### 10.1. Reactivity

Reactivity See the other subsections of this section for further details.

##### 10.2. Chemical stability

Stability Stable at normal ambient temperatures and when used as recommended. Stable under the prescribed storage conditions.

##### 10.3. Possibility of hazardous reactions

Possibility of hazardous reactions No potentially hazardous reactions known.

##### 10.4. Conditions to avoid

Conditions to avoid When exposed to air, this product will absorb moisture.

##### 10.5. Incompatible materials

Materials to avoid Avoid contact with strong oxidising agents. Strong alkalis.

##### 10.6. Hazardous decomposition products

Hazardous decomposition products Does not decompose when used and stored as recommended. Thermal decomposition or combustion products may include the following substances: Corrosive gases or vapours. Carbon monoxide (CO). Carbon dioxide (CO<sub>2</sub>). Nitrous gases (NO<sub>x</sub>). Sulphurous gases (SO<sub>x</sub>).

#### SECTION 11: Toxicological information

##### 11.1. Information on toxicological effects

###### Acute toxicity - oral

Summary Based on available data the classification criteria are not met.

###### Acute toxicity - dermal

Summary Based on available data the classification criteria are not met.

###### Acute toxicity - inhalation

Summary Based on available data the classification criteria are not met.

###### Skin corrosion/irritation

Summary Causes severe skin burns and eye damage.

###### Serious eye damage/irritation

Summary Causes serious eye damage.

###### Respiratory sensitisation

Summary Based on available data the classification criteria are not met.

###### Skin sensitisation

Summary Based on available data the classification criteria are not met.

###### Germ cell mutagenicity

Summary Based on available data the classification criteria are not met.

###### Carcinogenicity

Summary Based on available data the classification criteria are not met.

### 3-Methyl-1-(4-sulfofenyl)-2-pyrazolin-5-one

|  |  |
|--|--|
| <b>IARC carcinogenicity</b>                                      | None of the ingredients are listed or exempt.  |
| <b><u>Reproductive toxicity</u></b>                              |  |
| <b>Summary</b>   | Based on available data the classification criteria are not met.   |
| <b><u>Specific target organ toxicity - single exposure</u></b>   |  |
| <b>Summary</b>   | Based on available data the classification criteria are not met.   |
| <b><u>Specific target organ toxicity - repeated exposure</u></b> |  |
| <b>Summary</b>   | Based on available data the classification criteria are not met.   |
| <b><u>Aspiration hazard</u></b>                                  |  |
| <b>Summary</b>   | Not relevant. Solid.   |
| <b>General information</b>                                       | The severity of the symptoms described will vary dependent on the concentration and the length of exposure.  |
| <b>Inhalation</b>  | Corrosive to the respiratory tract. Symptoms following overexposure may include the following: Severe irritation of nose and throat.                         |
| <b>Ingestion</b>   | May cause chemical burns in mouth, oesophagus and stomach. Symptoms following overexposure may include the following: Severe stomach pain. Nausea, vomiting. |
| <b>Skin contact</b>  | Causes severe burns. Symptoms following overexposure may include the following: Pain or irritation. Redness. Blistering may occur.                           |
| <b>Eye contact</b>   | Causes serious eye damage. Symptoms following overexposure may include the following: Pain. Profuse watering of the eyes. Redness.                           |
| <b>Route of exposure</b>   | Ingestion Inhalation Skin and/or eye contact   |
| <b>Target organs</b>   | No specific target organs known.   |

## SECTION 12: Ecological information

### 12.1. Toxicity

#### Acute aquatic toxicity

**Summary** Based on available data the classification criteria are not met.

#### Chronic aquatic toxicity

**Summary** Harmful to aquatic life with long lasting effects.

### 12.2. Persistence and degradability

**Persistence and degradability** The degradability of the product is not known.

### 12.3. Bioaccumulative potential

**Bioaccumulative potential** No data available on bioaccumulation.

**Partition coefficient** No information available.

### 12.4. Mobility in soil

**Mobility** No data available.

### 12.5. Results of PBT and vPvB assessment

#### 12.6. Other adverse effects

**Other adverse effects** None known.

## SECTION 13: Disposal considerations

## 3-Methyl-1-(4-sulfophenyl)-2-pyrazolin-5-one

### 13.1. Waste treatment methods

|                            |  |
|----------------------------|--|
| <b>General information</b> | The generation of waste should be minimised or avoided wherever possible. Reuse or recycle products wherever possible. This material and its container must be disposed of in a safe way. When handling waste, the safety precautions applying to handling of the product should be considered. Care should be taken when handling emptied containers that have not been thoroughly cleaned or rinsed out. Empty containers or liners may retain some product residues and hence be potentially hazardous. |
| <b>Disposal methods</b>    | Do not empty into drains. Dispose of surplus products and those that cannot be recycled via a licensed waste disposal contractor. Waste, residues, empty containers, discarded work clothes and contaminated cleaning materials should be collected in designated containers, labelled with their contents. Incineration or landfill should only be considered when recycling is not feasible.   |

### SECTION 14: Transport information

|                |   |
|----------------|---|
| <b>General</b> | For limited quantity packaging/limited load information, consult the relevant modal documentation using the data shown in this section. |
|----------------|---|

#### 14.1. UN number

|                  |      |
|------------------|------|
| UN No. (ADR/RID) | 3261 |
| UN No. (IMDG)    | 3261 |
| UN No. (ICAO)    | 3261 |
| UN No. (ADN)     | 3261 |

#### 14.2. UN proper shipping name

|                                |   |
|--------------------------------|---|
| Proper shipping name (ADR/RID) | CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (3-Methyl-1-(4-sulfophenyl)-2-pyrazolin-5-one) |
| Proper shipping name (IMDG)    | CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (3-Methyl-1-(4-sulfophenyl)-2-pyrazolin-5-one) |
| Proper shipping name (ICAO)    | CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (3-Methyl-1-(4-sulfophenyl)-2-pyrazolin-5-one) |
| Proper shipping name (ADN)     | CORROSIVE SOLID, ACIDIC, ORGANIC, N.O.S. (3-Methyl-1-(4-sulfophenyl)-2-pyrazolin-5-one) |

#### 14.3. Transport hazard class(es)

|                             |    |
|-----------------------------|----|
| ADR/RID class               | 8  |
| ADR/RID classification code | C4 |
| ADR/RID label               | 8  |
| IMDG class                  | 8  |
| ICAO class/division         | 8  |
| ADN class                   | 8  |

#### Transport labels



#### 14.4. Packing group



### 3-Methyl-1-(4-sulfohenyl)-2-pyrazolin-5-one

|                       |    |
|-----------------------|----|
| ADR/RID packing group | II |
| IMDG packing group    | II |
| ICAO packing group    | II |
| ADN packing group     | II |

#### 14.5. Environmental hazards

Environmentally hazardous substance/marine pollutant

No.

#### 14.6. Special precautions for user

Always transport in closed containers that are upright and secure. Ensure that persons transporting the product know what to do in the event of an accident or spillage.

IMDG Code segregation group 1. Acids

EmS F-A, S-B

ADR transport category 2

Emergency Action Code 2X

Hazard Identification Number (ADR/RID) 80

Tunnel restriction code (E)

#### 14.7. Transport in bulk according to Annex II of MARPOL and the IBC Code

Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code Not applicable.

### SECTION 15: Regulatory information

#### 15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture

National regulations Health and Safety at Work etc. Act 1974 (as amended).  
The Carriage of Dangerous Goods and Use of Transportable Pressure Equipment Regulations 2009 (SI 2009 No. 1348) (as amended) ["CDG 2009"].  
EH40/2005 Workplace exposure limits.

#### 15.2. Chemical safety assessment

No chemical safety assessment has been carried out.

#### Inventories

##### EU - EINECS/ELINCS

None of the ingredients are listed or exempt.

### SECTION 16: Other information

### 3-Methyl-1-(4-sulfohenyl)-2-pyrazolin-5-one

|   |  |
|---|--|
| <b>Abbreviations and acronyms used in the safety data sheet</b> | ADR: European Agreement concerning the International Carriage of Dangerous Goods by Road.                  |
|   | ADN: European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways.      |
|   | RID: European Agreement concerning the International Carriage of Dangerous Goods by Rail.                  |
|   | IATA: International Air Transport Association.   |
|   | ICAO: Technical Instructions for the Safe Transport of Dangerous Goods by Air.                             |
|   | IMDG: International Maritime Dangerous Goods.  |
|   | CAS: Chemical Abstracts Service.   |
|   | ATE: Acute Toxicity Estimate.  |
|   | LC50: Lethal Concentration to 50 % of a test population.   |
|   | LD50: Lethal Dose to 50% of a test population (Median Lethal Dose).  |
|   | EC <sub>50</sub> : 50% of maximal Effective Concentration.   |
|   | PBT: Persistent, Bioaccumulative and Toxic substance.  |
|   | vPvB: Very Persistent and Very Bioaccumulative.  |
| <b>Classification abbreviations and acronyms</b>                | Eye Dam. = Serious eye damage  |
|   | Skin Corr. = Skin corrosion  |
|   | Aquatic Chronic = Hazardous to the aquatic environment (chronic)   |
| <b>Classification procedures according to SI 2019 No. 720</b>   | Eye Dam. 1 - H318: Skin Corr. 1B - H314: : Expert judgement. Aquatic Chronic 3 - H412: : Expert judgement. |
|   |  |
| <b>Training advice</b>  | Only trained personnel should use this material.   |
| <b>Revision date</b>  | 07/10/2022   |
| <b>Revision</b>   | 1  |
| <b>SDS number</b>   | 1621   |
| <b>Hazard statements in full</b>                                | H314 Causes severe skin burns and eye damage.  |
|   | H318 Causes serious eye damage.  |
|   | H412 Harmful to aquatic life with long lasting effects.  |

This information relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process. Such information is, to the best of the company's knowledge and belief, accurate and reliable as of the date indicated. However, no warranty, guarantee or representation is made to its accuracy, reliability or completeness. It is the user's responsibility to satisfy himself as to the suitability of such information for his own particular use.