

## SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 5.3 Revision Date 04.04.2013

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**SECTION 1: Identification of the substance/mixture and of the company/undertaking****1.1 Product identifiers**

Product name : 2,3-Dichloro-5,6-dicyano-*p*-benzoquinone

Product Number : D60400

Brand : Aldrich

REACH No. : A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.

CAS-No. : 84-58-2

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

Identified uses : Laboratory chemicals, Manufacture of substances

**1.3 Details of the supplier of the safety data sheet**

Company : Sigma-Aldrich Company Ltd.  
The Old Brickyard  
NEW ROAD, GILLINGHAM  
Dorset  
SP8 4XT  
UNITED KINGDOM

Telephone : +44 (0)1747 833000

Fax : +44 (0)1747 833313

E-mail address : eurtechserv@sial.com

**1.4 Emergency telephone number**

Emergency Phone # : +44 (0)1747 833100

**SECTION 2: Hazards identification****2.1 Classification of the substance or mixture****Classification according to Regulation (EC) No 1272/2008**

Acute toxicity, Oral (Category 3), H301

For the full text of the H-Statements mentioned in this Section, see Section 16.

**Classification according to EU Directives 67/548/EEC or 1999/45/EC**

T Toxic R25, R29

For the full text of the R-phrases mentioned in this Section, see Section 16.

**2.2 Label elements****Labelling according Regulation (EC) No 1272/2008**

Pictogram



Signal word Danger

Hazard statement(s)  
H301 Toxic if swallowed.

Precautionary statement(s)  
P301 + P310 IF SWALLOWED: Immediately call a POISON CENTER or doctor/

physician.

Supplemental Hazard information (EU)

EUH029

Contact with water liberates toxic gas.

## 2.3 Other hazards - none

### SECTION 3: Composition/information on ingredients

#### 3.1 Substances

Formula :  $C_8Cl_2N_2O_2$   
Molecular Weight : 227.00 g/mol  
CAS-No. : 84-58-2  
EC-No. : 201-542-2

#### Hazardous ingredients according to Regulation (EC) No 1272/2008

Component	Classification	Concentration
<b>4,5-Dichloro-3,6-dioxocyclohexa-1,4-diene-1,2-dicarbonitrile</b>		
	Acute Tox. 3; H301, EUH029	-

#### Hazardous ingredients according to Directive 1999/45/EC

Component	Classification	Concentration
<b>4,5-Dichloro-3,6-dioxocyclohexa-1,4-diene-1,2-dicarbonitrile</b>		
	T, R25 - R29	-

For the full text of the H-Statements and R-Phrases mentioned in this Section, see Section 16

### SECTION 4: First aid measures

#### 4.1 Description of first aid measures

##### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.

##### If inhaled

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

##### In case of skin contact

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

##### In case of eye contact

Flush eyes with water as a precaution.

##### If swallowed

Never give anything by mouth to an unconscious person. Rinse mouth with water. 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

Dry powder

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

Carbon oxides, nitrogen oxides (NO<sub>x</sub>), Hydrogen chloride gas, Hydrogen cyanide (hydrocyanic acid)

#### 5.3 Advice for firefighters

Wear self contained breathing apparatus for fire fighting if necessary.

#### 5.4 Further information

no data available

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## SECTION 6: Accidental release measures

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

Wear respiratory protection. Avoid dust formation. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Evacuate personnel to safe areas. Avoid breathing dust.  
For personal protection see section 8.

### 6.2 Environmental precautions

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

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

Pick up and arrange disposal without creating dust. Sweep up and shovel. Do not flush with water. Keep in suitable, closed containers for disposal.

### 6.4 Reference to other sections

For disposal see section 13.

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## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

Avoid contact with skin and eyes. Avoid formation of dust and aerosols.  
Provide appropriate exhaust ventilation at places where dust is formed.  
For precautions see section 2.2.

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

Store in cool place. Keep container tightly closed in a dry and well-ventilated place.  
Never allow product to get in contact with water during storage.

Recommended storage temperature: 2 - 8 °C

Moisture sensitive.

### 7.3 Specific end use(s)

A part from the uses mentioned in section 1.2 no other specific uses are stipulated

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## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

#### Components with workplace control parameters

Contains no substances with occupational exposure limit values.

### 8.2 Exposure controls

#### Appropriate engineering controls

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

#### Personal protective equipment

##### Eye/face protection

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

##### Skin protection

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. 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.

Full contact

Material: Nitrile rubber

Minimum layer thickness: 0.11 mm

Break through time: 480 min

Material tested: Dermatrill® (KCL 740 / Aldrich Z677272, Size M)

Splash contact  
Material: Nitrile rubber  
Minimum layer thickness: 0.11 mm  
Break through time: 480 min  
Material tested: Dermatril® (KCL 740 / Aldrich Z677272, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de,  
test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

### **Body Protection**

Complete suit protecting against chemicals, The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

### **Respiratory protection**

Where risk assessment shows air-purifying respirators are appropriate use a full-face particle respirator type N100 (US) or type P3 (EN 143) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

### **Control of environmental exposure**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

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## **SECTION 9: Physical and chemical properties**

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

- |   |  |
|---|--|
| a) Appearance                                   | Form: crystalline<br>Colour: dark yellow |
| b) Odour  | no data available                        |
| c) Odour Threshold                              | no data available                        |
| d) pH   | no data available                        |
| e) Melting point/freezing point                 | Melting point/range: 210 - 215 °C - dec. |
| f) Initial boiling point and boiling range      | no data available                        |
| g) Flash point                                  | no data available                        |
| h) Evaporation rate                             | no data available                        |
| i) Flammability (solid, gas)                    | no data available                        |
| j) Upper/lower flammability or explosive limits | no data available                        |
| k) Vapour pressure                              | no data available                        |
| l) Vapour density                               | no data available                        |
| m) Relative density                             | no data available                        |
| n) Water solubility                             | no data available                        |
| o) Partition coefficient: n-octanol/water       | no data available                        |
| p) Auto-ignition temperature                    | no data available                        |
| q) Decomposition                                | no data available                        |

temperature

- r) Viscosity no data available
- s) Explosive properties no data available
- t) Oxidizing properties no data available

## 9.2 Other safety information

no data available

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

no data available

### 10.2 Chemical stability

Stable under recommended storage conditions.

### 10.3 Possibility of hazardous reactions

Reacts violently with water.

### 10.4 Conditions to avoid

In the presence of water this material decomposes to hydrogen cyanide, therefore, most reactions with this reagent should be carried out under anhydrous conditions.

Exposure to moisture.

### 10.5 Incompatible materials

Strong acids, Strong bases, Strong oxidizing agents, Strong reducing agents

### 10.6 Hazardous decomposition products

Other decomposition products - no data available

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute toxicity

LD50 Oral - rat - 82 mg/kg

#### Skin corrosion/irritation

no data available

#### Serious eye damage/eye irritation

no data available

#### Respiratory or skin sensitisation

no data available

#### Germ cell mutagenicity

no data available

#### Carcinogenicity

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

#### Reproductive 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

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**SECTION 12: Ecological information**

- 12.1 Toxicity**  
no data available
- 12.2 Persistence and degradability**  
no data available
- 12.3 Bioaccumulative potential**  
no data available
- 12.4 Mobility in soil**  
no data available
- 12.5 Results of PBT and vPvB assessment**  
PBT/vPvB assessment not available as chemical safety assessment not required/not conducted
- 12.6 Other adverse effects**  
no data available

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**SECTION 13: Disposal considerations****13.1 Waste treatment methods****Product**

Offer surplus and non-recyclable solutions to a licensed disposal company. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber.

**Contaminated packaging**

Dispose of as unused product.

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**SECTION 14: Transport information**

- 14.1 UN number**  
ADR/RID: 3439                      IMDG: 3439                      IATA: 3439
- 14.2 UN proper shipping name**  
ADR/RID: NITRILES, TOXIC, SOLID, N.O.S. (4,5-Dichloro-3,6-dioxocyclohexa-1,4-diene-1,2-dicarbonitrile)  
IMDG: NITRILES, TOXIC, SOLID, N.O.S. (4,5-Dichloro-3,6-dioxocyclohexa-1,4-diene-1,2-dicarbonitrile)  
IATA: Nitriles, solid, toxic, n.o.s. (4,5-Dichloro-3,6-dioxocyclohexa-1,4-diene-1,2-dicarbonitrile)
- 14.3 Transport hazard class(es)**  
ADR/RID: 6.1                      IMDG: 6.1                      IATA: 6.1
- 14.4 Packaging group**  
ADR/RID: III                      IMDG: III                      IATA: III
- 14.5 Environmental hazards**  
ADR/RID: no                      IMDG Marine pollutant: no                      IATA: no
- 14.6 Special precautions for user**  
no data available

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**SECTION 15: Regulatory information**

This safety datasheet complies with the requirements of Regulation (EC) No. 1907/2006.

- 15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture**  
no data available
- 15.2 Chemical Safety Assessment**  
For this product a chemical safety assessment was not carried out

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**SECTION 16: Other information****Full text of H-Statements referred to under sections 2 and 3.**

Acute Tox.	Acute toxicity
EUH029	Contact with water liberates toxic gas.
H301	Toxic if swallowed.

**Full text of R-phrases referred to under sections 2 and 3**

T	Toxic
R25	Toxic if swallowed.
R29	Contact with water liberates toxic gas.

**Further information**

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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](http://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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