

# SAFETY DATA SHEET

Version 6.16  
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## SECTION 1. IDENTIFICATION

### 1.1 Product identifiers

Product name : Pyrocatechol  
Product Number : C9510  
Brand : Sigma-Aldrich  
Index-No. : 604-016-00-4  
CAS-No. : 120-80-9

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

Identified uses : Laboratory chemicals, Synthesis of substances  
Uses advised against : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

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

Company : Sigma-Aldrich Inc.  
3050 SPRUCE ST  
ST. LOUIS MO 63103  
UNITED STATES  
Telephone : +1 314 771-5765  
Fax : +1 800 325-5052

### 1.4 Emergency telephone

Emergency Phone # : 800-424-9300 CHEMTREC (USA) +1-703-527-3887 CHEMTREC (International) 24 Hours/day; 7 Days/week

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## SECTION 2. HAZARDS IDENTIFICATION

### GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Acute toxicity (Oral) : Category 3

Acute toxicity (Dermal) : Category 3  
 Skin irritation : Category 2  
 Serious eye damage : Category 1  
 Skin sensitization : Category 1  
 Germ cell mutagenicity : Category 2  
 Carcinogenicity : Category 1B  
 Short-term (acute) aquatic hazard : Category 2

**GHS label elements**

Hazard pictograms : 

Signal Word : Danger

Hazard Statements : H301 + H311 Toxic if swallowed or in contact with skin.  
 H315 Causes skin irritation.  
 H317 May cause an allergic skin reaction.  
 H318 Causes serious eye damage.  
 H341 Suspected of causing genetic defects.  
 H350 May cause cancer.  
 H401 Toxic to aquatic life.

Precautionary Statements : **Prevention:**  
 P201 Obtain special instructions before use.  
 P202 Do not handle until all safety precautions have been read and understood.  
 P261 Avoid breathing dust.  
 P264 Wash skin thoroughly after handling.  
 P270 Do not eat, drink or smoke when using this product.  
 P272 Contaminated work clothing must not be allowed out of the workplace.  
 P273 Avoid release to the environment.  
 P280 Wear protective gloves/ protective clothing/ eye protection/ face protection.

**Response:**  
 P301 + P310 + P330 IF SWALLOWED: Immediately call a POISON CENTER/ doctor. Rinse mouth.  
 P302 + P352 + P312 IF ON SKIN: Wash with plenty of water. Call a POISON CENTER/ doctor if you feel unwell.  
 P305 + P351 + P338 + P310 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact

lenses, if present and easy to do. Continue rinsing.  
Immediately call a POISON CENTER/ doctor.  
P308 + P313 IF exposed or concerned: Get medical advice/ attention.  
P333 + P313 If skin irritation or rash occurs: Get medical advice/ attention.  
P362 Take off contaminated clothing and wash before reuse.

**Storage:**

P405 Store locked up.

**Disposal:**

P501 Dispose of contents/ container to an approved waste disposal plant.

**Other hazards**

None known.

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**SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS**

Substance / Mixture : Substance

**Components**

Chemical name	CAS-No.	Concentration (% w/w)
Pyrocatechol	120-80-9	>= 90 - <= 100

Actual concentration is withheld as a trade secret

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**SECTION 4. FIRST AID MEASURES**

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

If inhaled : After inhalation: fresh air. Call in physician.

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

In case of eye contact : After eye contact: rinse out with plenty of water.  
Immediately call in ophthalmologist.  
Remove contact lenses.

If swallowed : If swallowed: give water to drink (two glasses at most). Seek medical advice immediately. In exceptional cases only, if medical care is not available within one hour, induce vomiting (only in persons who are wide awake and fully conscious), administer activated charcoal (20 - 40 g in a 10% slurry) and consult a doctor as quickly as possible.

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
Protection of first-aiders	: For personal protection see section 8.
Notes to physician	: No data available

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## SECTION 5. FIRE-FIGHTING MEASURES

Suitable extinguishing media	: Water Foam Carbon dioxide (CO <sub>2</sub> ) Dry powder
Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
Specific hazards during fire fighting	: Combustible.  Vapors are heavier than air and may spread along floors.  Forms explosive mixtures with air on intense heating.  Development of hazardous combustion gases or vapours possible in the event of fire.
Hazardous combustion products	: Carbon oxides
Specific extinguishing methods	: No data available
Further information	: Prevent fire extinguishing water from contaminating surface water or the ground water system.
Special protective equipment for fire-fighters	: Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

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## SECTION 6. ACCIDENTAL RELEASE MEASURES

- Personal precautions, protective equipment and emergency procedures : Advice for non-emergency personnel:  
Avoid generation and inhalation of dusts in all circumstances.  
Avoid substance contact.  
Ensure adequate ventilation.  
Evacuate the danger area, observe emergency procedures, consult an expert.  
Advice for emergency responders:  
For personal protection see section 8.
- Environmental precautions : Do not let product enter drains.
- Methods and materials for containment and cleaning up : Cover drains. Collect, bind, and pump off spills.  
Observe possible material restrictions (see sections 7 and 10).  
Take up carefully. Dispose of properly. Clean up affected area.  
Avoid generation of dusts.

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## SECTION 7. HANDLING AND STORAGE

For precautions see section 2.2.

- Advice on safe handling : Work under hood. Do not inhale substance/mixture.
- Further information on storage conditions : Tightly closed.  
Dry.  
Keep in a well-ventilated place.  
Keep locked up or in an area accessible only to qualified or authorized persons.
- Storage class : 6.1C, Combustible, acute toxic Cat.3 / toxic compounds or compounds which causing chronic effects
- Recommended storage temperature : Recommended storage temperature see product label.
- Further information on storage stability : Store under inert gas.  
Air and light sensitive.

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## SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

### Ingredients with workplace control parameters

Components	CAS-No.	Value type (Form of exposure)	Control parameters / Permissible concentra-	Basis

			tion	
Pyrocatechol	120-80-9	TWA	5 ppm	ACGIH
		TWA	5 mg/m <sup>3</sup>	OSHA P0
		STEL	20 ppm	OSHA P0
		TWA	5 ppm 20 mg/m <sup>3</sup>	NIOSH REL

### Biological occupational exposure limits

Components	CAS-No.	Control parameters	Biological specimen	Sampling time	Permissible concentration	Basis
Pyrocatechol	120-80-9	Methemoglobin	In blood	During or at the end of the shift	5 % Hb	ACGIH BEI

**Engineering measures** : No data available

### Personal protective equipment

Respiratory protection : required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: : Filter type P3

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

#### Hand protection

Material : Nitrile rubber  
 Break through time : 480 min  
 Glove thickness : 0.11 mm  
 Protective index : Full contact  
 Manufacturer : KCL 741 Dermatril® L

Material : Nitrile rubber  
 Break through time : 480 min  
 Glove thickness : 0.11 mm  
 Protective index : Splash contact  
 Manufacturer : KCL 741 Dermatril® L

Remarks : This recommendation applies only to the product stated in the safety data sheet, supplied by us and

for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

- Eye protection : Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).  
Tightly fitting safety goggles
- Skin and body protection : protective clothing
- Hygiene measures : Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.

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## SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

- Appearance : powder
- Color : brown
- Odor : No data available
- Odor Threshold : No data available  
pH : No data available
- Melting point/ range : 212 - 217 °F / 100 - 103 °C  
Method: lit.
- Boiling point/boiling range : 473 °F / 245 °C  
Method: lit.
- Flash point : 261 °F / 127 °C  
Method: closed cup
- Evaporation rate : No data available
- Burning rate : No data available
- Self-ignition : 950 °F / 510 °C
- Upper explosion limit /  
Upper flammability limit : No data available
- Lower explosion limit / : Lower explosion limit

Lower flammability limit	: 1.97 %(V)
Vapor pressure	: 13 hPa (244.9 °F / 118.3 °C) 1 hPa (167 °F / 75 °C)
Relative vapor density	: No data available
Relative density	: No data available
Density	: 1.34 g/cm <sup>3</sup> (59 °F / 15 °C)
Water solubility	: No data available
Partition coefficient: n-octanol/water	: log Pow: 0.88 (77 °F / 25 °C) Method: OECD Test Guideline 117 Bioaccumulation is not expected.
Autoignition temperature	: 950 °F / 510 °C
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: Not classified as explosive.
Oxidizing properties	: none
Molecular weight	: 110.11 g/mol
Particle characteristics Particle size	: No data available

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## SECTION 10. STABILITY AND REACTIVITY

Reactivity	: Forms explosive mixtures with air on intense heating.  A range from approx. 15 Kelvin below the flash point is to be rated as critical.  The following applies in general to flammable organic substances and mixtures: in correspondingly fine distribution, when whirled up a dust explosion potential may generally be assumed.
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Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	: Risk of explosion with: Oxidizing agents nitric acid (conc.) can decompose violently in contact with: Exothermic reaction with: Bases Acid anhydrides alkali compounds
Conditions to avoid	: Strong heating.
Incompatible materials	: No data available
Hazardous decomposition products	: 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 - male - 300 mg/kg

Remarks: (ECHA)

Inhalation: No data available

LD50 Dermal - Rat - male and female - 600 mg/kg  
(OECD Test Guideline 402)

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

#### Skin corrosion/irritation

Skin - Rabbit

Result: Irritating to skin. - 24 h

(Draize Test)

#### Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye damage. - 24 - 72 h

(Draize Test)

Remarks: (ECHA)

#### Respiratory or skin sensitization

Freund's complete adjuvant test - Guinea pig

Result: positive

Remarks: (ECHA)

#### Germ cell mutagenicity

Suspected of causing genetic defects.

Test Type: Ames test

Test system: Salmonella typhimurium

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: In vitro mammalian cell gene mutation test

Test system: mouse lymphoma cells  
Metabolic activation: without metabolic activation  
Method: OECD Test Guideline 476  
Result: positive

Test Type: comet assay  
Species: Rat

Application Route: Oral

Result: positive  
Remarks: (ECHA)

### **Carcinogenicity**

Presumed to have carcinogenic potential for humans

IARC: 2B - Group 2B: Possibly carcinogenic to humans (Pyrocatechol)

NTP: No ingredient of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.

OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

### **Reproductive toxicity**

No data available

### **Specific target organ toxicity - single exposure**

No data available

### **Specific target organ toxicity - repeated exposure**

No data available

### **Aspiration hazard**

No data available

## **11.2 Additional Information**

RTECS: UX1050000

Cough, Shortness of breath, Headache, Nausea, Vomiting

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

Stomach - Irregularities - Based on Human Evidence

Stomach - Irregularities - Based on Human Evidence

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## **SECTION 12. ECOLOGICAL INFORMATION**

### **Ecotoxicity**

#### **Components:**

#### **Pyrocatechol:**

Toxicity to fish : LC50 (Pimephales promelas (fathead minnow)): 9.22

mg/l  
End point: mortality  
Exposure time: 96 h  
Test Type: flow-through test  
Analytical monitoring: yes  
Method: OECD Test Guideline 203

Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia magna (Water flea)): 1.09 mg/l  
End point: Immobilization  
Exposure time: 48 h  
Test Type: semi-static test  
Analytical monitoring: yes  
Method: OECD Test Guideline 202  
GLP: yes

Toxicity to algae/aquatic plants : ErC50 (Chlorella vulgaris (Fresh water algae)): 22 mg/l  
Exposure time: 96 h  
Method: OECD Test Guideline 201

### **Persistence and degradability**

#### **Components:**

##### **Pyrocatechol:**

Biodegradability : aerobic  
Inoculum: activated sludge, non-adapted  
Concentration: 100 mg/l  
Result: Readily biodegradable.  
Biodegradation: 96 %  
Exposure time: 14 d  
Method: OECD Test Guideline 301C

### **Bioaccumulative potential**

#### **Components:**

##### **Pyrocatechol:**

Partition coefficient: n-octanol/water : log Pow: 0.88 (77 °F / 25 °C)  
Method: OECD Test Guideline 117  
Remarks: Bioaccumulation is not expected.

### **Mobility in soil**

No data available

### **Other adverse effects**

#### **Product:**

Ozone-Depletion Potential : Regulation: 40 CFR Protection of Environment; Part 82  
Protection of Stratospheric Ozone - CAA Section 602  
Class I Substances  
Remarks: This product neither contains, nor was

manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B).

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## SECTION 13. DISPOSAL CONSIDERATIONS

### Disposal methods

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

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## SECTION 14. TRANSPORT INFORMATION

### International Regulations

#### IATA-DGR

UN/ID No. : UN 2811  
Proper shipping name : Toxic solid, organic, n.o.s.  
(Pyrocatechol)  
Class : 6.1  
Packing group : III  
Labels : Division 6.1 - Toxic substances  
Packing instruction (cargo : 677  
aircraft)  
Packing instruction (passenger aircraft) : 670

#### IMDG-Code

UN number : UN 2811  
Proper shipping name : TOXIC SOLID, ORGANIC, N.O.S.  
(Pyrocatechol)  
Class : 6.1  
Packing group : III  
Labels : 6.1  
EmS Code : F-A, S-A  
Marine pollutant : no

#### Transport in bulk according to Annex II of MARPOL 73/78 and the IBC Code

Not applicable for product as supplied.

### National regulation

#### 49 CFR Road

UN/ID/NA number : UN 2811  
Proper shipping name : Toxic solids, organic, n.o.s.  
(Pyrocatechol)  
Class : 6.1  
Packing group : III  
Labels : Division 6.1 - Toxic substances  
ERG Code : 154

Marine pollutant : no

Poison Inhalation Hazard : No

### Special precautions for user

The transport classification(s) provided herein are for informational purposes only, and solely based upon the properties of the unpackaged material as it is described within this Safety Data Sheet. Transportation classifications may vary by mode of transportation, package sizes, and variations in regional or country regulations.

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## SECTION 15. REGULATORY INFORMATION

### CERCLA Reportable Quantity

Components	CAS-No.	Component RQ (lbs)	Calculated product RQ (lbs)
Pyrocatechol	120-80-9	100	100

### SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

### SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

This material does not contain any components with a section 302 EHS TPQ.

**SARA 311/312 Hazards** : Acute Health Hazard  
Chronic Health Hazard

**SARA 313** : The following components are subject to reporting levels established by SARA Title III, Section 313:

Pyrocatechol 120-80-9 >= 90 - <= 100 %

### Clean Air Act

This product neither contains, nor was manufactured with a Class I or Class II ODS as defined by the U.S. Clean Air Act Section 602 (40 CFR 82, Subpt. A, App.A + B). The following chemical(s) are listed as HAP under the U.S. Clean Air Act, Section 112 (40 CFR 61):

Pyrocatechol 120-80-9 >= 90 - <= 100 %

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 112(r) for Accidental Release Prevention (40 CFR 68.130, Subpart F).

This product does not contain any chemicals listed under the U.S. Clean Air Act Section 111 SOCOMI Intermediate or Final VOC's (40 CFR 60.489).

### Clean Water Act

This product does not contain any Hazardous Substances listed under the U.S. CleanWater Act, Section 311, Table 116.4A.

This product does not contain any Hazardous Chemicals listed under the U.S. Clean-Water Act, Section 311, Table 117.3.

This product does not contain any toxic pollutants listed under the U.S. Clean Water Act Section 307

This product does not contain any priority pollutants related to the U.S. Clean Water Act

### **US State Regulations**

#### **Massachusetts Right To Know**

Pyrocatechol 120-80-9

#### **Pennsylvania Right To Know**

Pyrocatechol 120-80-9

#### **Maine Chemicals of High Concern**

Product does not contain any listed chemicals

#### **Vermont Chemicals of High Concern**

Product does not contain any listed chemicals

#### **Washington Chemicals of High Concern**

Product does not contain any listed chemicals

#### **California Prop. 65**

WARNING: This product can expose you to chemicals including Pyrocatechol, which is/are known to the State of California to cause cancer. For more information go to [www.P65Warnings.ca.gov](http://www.P65Warnings.ca.gov).

#### **The ingredients of this product are reported in the following inventories:**

TSCA : All substances listed as active on the TSCA inventory

#### **TSCA list**

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

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## **SECTION 16. OTHER INFORMATION**

### **Full text of other abbreviations**

ACGIH : USA. ACGIH Threshold Limit Values (TLV)  
ACGIH BEI : ACGIH - Biological Exposure Indices (BEI)  
NIOSH REL : USA. NIOSH Recommended Exposure Limits  
OSHA P0 : USA. Table Z-1-A Limits for Air Contaminants (1989 vacated values)  
ACGIH / TWA : 8-hour, time-weighted average  
NIOSH REL / TWA : Time-weighted average concentration for up to a 10-hour workday during a 40-hour workweek  
OSHA P0 / TWA : 8-hour time weighted average  
OSHA P0 / STEL : Short-term exposure limit

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT -

Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; ERG - Emergency Response Guide; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

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The Merck logo, consisting of the word "MERCK" in a bold, red, sans-serif font.

