

## Chemical Safety Data Sheet MSDS / SDS

**5-METHYL-2-[(1R,6R)-3-METHYL-6-(1-METHYLETHENYL)-2-CYCLOHEXEN-1-YL]-1,3-BENZENEDIOL**

Revision Date:2026-05-31 Revision Number:1

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

Product name : 5-METHYL-2-[(1R,6R)-3-METHYL-6-(1-METHYLETHENYL)-2-CYCLOHEXEN-1-YL]-1,3-BENZENEDIOL

CBnumber : CB4108553

CAS : 35482-50-9

Synonyms : 1,3-Benzenediol, 5-methyl-2-[(1R,6R)-3-methyl-6-(1-methylethenyl)-2-cyclohexen-1-yl]-,o-1821

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

Relevant identified uses : For R&D use only. Not for medicinal, household or other use.

Uses advised against : none

**Company Identification**

Company : Chemicalbook

Address : Building 1, Huihuang International, Shangdi 10th Street, Haidian District, Beijing

Telephone : 010-86108875

**SECTION 2: Hazards identification****GHS Label elements, including precautionary statements**

Symbol(GHS)



Signal word

Danger

**Precautionary statements**

P210 Keep away from heat/sparks/open flames/hot surfaces. — No smoking.

P233 Keep container tightly closed.

P240 Ground/bond container and receiving equipment.

P241 Use explosion-proof electrical/ventilating/lighting/.../equipment.

P242 Use only non-sparking tools.

P243 Take precautionary measures against static discharge.

P261 Avoid breathing dust/fume/gas/mist/vapours/spray.

P264 Wash skin thoroughly after handling.

P270 Do not eat, drink or smoke when using this product.

P271 Use only outdoors or in a well-ventilated area.

P280 Wear protective gloves/protective clothing/eye protection/face protection.

P301+P312 IF SWALLOWED: call a POISON CENTER or doctor/physician IF you feel unwell.

P303+P361+P353 IF ON SKIN (or hair): Remove/Take off Immediately all contaminated clothing. Rinse SKIN with water/shower.

P304+P340 IF INHALED: Remove victim to fresh air and Keep at rest in a position comfortable for breathing.

P305+P351+P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do.

Continuerinsing.

P321 Specific treatment (see ... on this label).

P330 Rinse mouth.

P337+P313 IF eye irritation persists: Get medical advice/attention.

P370+P378 In case of fire: Use ... for extinction.

P403+P235 Store in a well-ventilated place. Keep cool.

P501 Dispose of contents/container to.....

#### **Hazard statements**

H225 Highly Flammable liquid and vapour

H319 Causes serious eye irritation

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## SECTION 3: Composition/information on ingredients

### **Substance**

Product name	: 5-METHYL-2-[(1R,6R)-3-METHYL-6-(1-METHYLETHENYL)-2-CYCLOHEXEN-1-YL]-1,3-BENZENEDIOL
Synonyms	: 1,3-Benzenediol, 5-methyl-2-[(1R,6R)-3-methyl-6-(1-methylethenyl)-2-cyclohexen-1-yl]-,o-1821
CAS	: 35482-50-9
MF	: C17H22O2
MW	: 258.36

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## SECTION 4: First aid measures

### **Description of first aid measures**

#### **General information**

Immediately remove any clothing soiled by the product.

Symptoms of poisoning may even occur after several hours; therefore medical observation for at least 48 hours after the accident.

#### **After inhalation**

Supply fresh air. If required, provide artificial respiration. Keep patient warm. Consult doctor if symptoms persist.

In case of unconsciousness place patient stably in side position for transportation.

#### **After skin contact**

Immediately rinse with water.

#### **After eye contact**

Rinse opened eye for several minutes under running water. If symptoms persist, consult a doctor.

### After swallowing

Immediately call a doctor.

### Information for doctor

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

No further relevant information available.

### Indication of any immediate medical attention and special treatment needed

No further relevant information available.

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## SECTION 5: Firefighting measures

### Extinguishing media

#### Suitable extinguishing agents

CO<sub>2</sub>, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

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

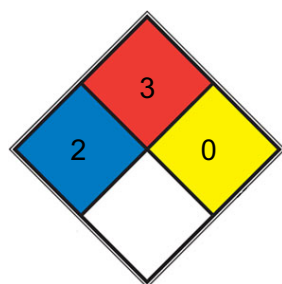
No further relevant information available.

#### Advice for firefighters

#### Protective equipment

Mouth respiratory protective device.

#### NFPA 704



**HEALTH 2** Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury (e.g. [diethyl ether](#), ammonium phosphate, iodine)

**FIRE 3** Liquids and solids (including finely divided suspended solids) that can be ignited under almost all ambient temperature conditions. Liquids having a flash point below 22.8 °C (73 °F) and having a boiling point at or above 37.8 °C (100 °F) or having a flash point between 22.8 and 37.8 °C (73 and 100 °F). (e.g. gasoline, [acetone](#))

**REACT 0** Normally stable, even under fire exposure conditions, and is not reactive with water (e.g. helium, [N<sub>2</sub>](#))

**SPEC.**

## SECTION 6: Accidental release measures

### Personal precautions, protective equipment and emergency procedures

Wear protective equipment. Keep unprotected persons away.

### Environmental precautions

Dilute with plenty of water.

Do not allow to enter sewers/ surface or ground water.

### Methods and material for containment and cleaning up

Absorb with liquid-binding material (sand, diatomite, acid binders, universal binders, sawdust).

Dispose contaminated material as waste according to item 13.

Ensure adequate ventilation.

### Reference to other sections

See Section 7 for information on safe handling.

See Section 8 for information on personal protection equipment.

See Section 13 for disposal information.

### Protective Action Criteria for Chemicals

#### PAC-1

75-05-8 Acetonitrile 13 ppm

#### PAC-2

75-05-8 Acetonitrile 50 ppm

#### PAC-3

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## SECTION 7: Handling and storage

### Handling

#### Precautions for safe handling

Ensure good ventilation/exhaustion at the workplace.

Prevent formation of aerosols.

#### Information about protection against explosions and fires

Keep ignition sources away - Do not smoke.

Protect against electrostatic charges.

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

## Storage

Store in accordance with information listed on the product insert.

## Requirements to be met by storerooms and receptacles

Store in a cool location.

## Information about storage in one common storage facility

Not required.

## Further information about storage conditions

Keep receptacle tightly sealed.

Store in cool, dry conditions in well sealed receptacles.

## Specific end use(s)

No further relevant information available.

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# SECTION 8: Exposure controls/personal protection

## Additional information about design of technical systems

No further data; see item 7.

## Control parameters

Components with limit values that require monitoring at the workplace:

75-05-8 Acetonitrile	
PEL	Long-term value: 70 mg/m <sup>3</sup> , 40 ppm
REL	Long-term value: 34 mg/m <sup>3</sup> , 20 ppm
TLV	Long-term value: 20 ppm Skin, A4

## Additional information

The lists that were valid during the creation were used as basis.

## Exposure controls

### Personal protective equipment

### General protective and hygienic measures

Keep away from foodstuffs, beverages and feed.

Immediately remove all soiled and contaminated clothing.

Wash hands before breaks and at the end of work.

Avoid contact with the eyes.

Avoid contact with the eyes and skin.

## Breathing equipment

In case of brief exposure or low pollution use respiratory filter device. In case of intensive or longer exposure use respiratory protective device that is independent of circulating air.

## Protection of hands

Protective gloves

The glove material has to be impermeable and resistant to the product/ the substance/ the preparation.

Due to missing tests no recommendation to the glove material can be given for the product/ the preparation/ the chemical mixture.

Selection of the glove material on consideration of the penetration times, rates of diffusion and the degradation

## Material of gloves

The selection of the suitable gloves does not only depend on the material, but also on further marks of quality and varies from manufacturer to manufacturer. As the product is a preparation of several substances, the resistance of the glove material can not be calculated in advance and has therefore to be checked prior to the application.

## Penetration time of glove material

The exact break through time has to be found out by the manufacturer of the protective gloves and has to be observed.

## Eye protection

Tightly sealed goggles

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# SECTION 9: Physical and chemical properties

## Information on basic physicochemical properties

### Appearance

### Physical State

Liquid

### Color

According to product specification

### Odor

Aromatic

### Structural Formula

C<sub>17</sub>H<sub>22</sub>O<sub>2</sub>

### Molecular Weight

258.4 g/mol

### Odor Threshold

Not determined.

**Formulation**

A 1mg/mL solution in acetonitrile

**pH**

Not determined.

**Change in condition****Melting point/Melting range**

-46 °C (-50.8 °F)

**Boiling point/Boiling range**

81 °C (177.8 °F)

**Flash point**

5 °C (41 °F)

**Flammability (solid,gas)**

Highly flammable.

**Auto igniting**

525 °C (977 °F)

**Decomposition temperature**

Not determined.

**Ignition temperature**

Product is not selfigniting.

**Danger of explosion**

Product is not explosive. However, formation of explosive air/ vapor mixtures are possible.

**Explosion limits**

Lower: 4.4 Vol %

Upper: 16 Vol %

**Vapor Pressure at 20 °C (68 °F)**

97 hPa (72.8 mm Hg)

**Density at 20 °C (68 °F)**

0.7822 g/cm<sup>3</sup> (6.52746 lbs/gal)

**Relative Density**

1.073±0.06 g/cm<sup>3</sup>(Predicted)

**Vapor Density**

Not determined.

### **Evaporation Rate**

Not determined.

### **Solubility in / Miscibility with**

≤30mg/ml in ethanol;30mg/ml in DMSO;30mg/ml in dimethyl formamide

### **Water**

Fully miscible.

### **Partition coefficient (n-octanol/water)**

Not determined.

### **Viscosity**

#### **Dynamic**

at 20 °C (68 °F): 0.39 mPas

#### **Kinematic**

Not determined.

### **VOC content**

0.00 % 0.0 g/l / 0.00 lb/gal

### **Solids content**

0.1 %

### **Other information**

No information available

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## SECTION 10: Stability and reactivity

### **Reactivity**

No further relevant information available.

### **Chemical stability**

#### **Thermal decomposition / conditions to be avoided**

No decomposition if used according to specifications.

#### **Possibility of hazardous reactions**

No dangerous reactions known.

#### **Conditions to avoid**

No further relevant information available.

## Incompatible materials

No further relevant information available.

## Hazardous decomposition products

No dangerous decomposition products known.

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## SECTION 11: Toxicological information

### Information on toxicological effects

#### Acute toxicity

LD/LC50 values that are relevant for classification:

Substance / Estimate	Route	Endpoint	Value
ATE (Acute Toxicity Estimate)	Oral	LD50	501 mg/kg
ATE (Acute Toxicity Estimate)	Dermal	LD50	1,101 mg/kg
ATE (Acute Toxicity Estimate)	Inhalative	LC50/4 h	11 mg/l
75-05-8 Acetonitrile	Oral	TDLO	64 ml/kg (man)
75-05-8 Acetonitrile	Oral	LD50	2,460 mg/kg (rat)
75-05-8 Acetonitrile	Dermal	LD50	980 mg/kg (rabbit)
75-05-8 Acetonitrile	Inhalative	LC50/4 h	7,551 mg/m <sup>3</sup> (rat)
75-05-8 Acetonitrile	Inhalative	LC50	7,551 mg/m <sup>3</sup> /8h (rat) TCLO 160 mg/m <sup>3</sup> /4h (hmn) Irritation of eyes Irritation 100 µl/24 hr (rabbit) Irritation 100 il/24 hr (rabbit)

#### Primary irritant effect

##### on the skin

No irritant effect.

##### on the eye

Irritating effect.

#### Sensitization

No sensitizing effects known.

#### Additional toxicological information

The product shows the following dangers according to internally approved calculation methods for preparations

Harmful

Irritant

#### Carcinogenic categories

**IARC (International Agency for Research on Cancer)**

None of the ingredients is listed.

**NTP (National Toxicology Program)**

None of the ingredients is listed.

**OSHA-Ca (Occupational Safety & Health Administration)**

None of the ingredients is listed.

**SECTION 12: Ecological information****Results of PBT and vPvB assessment****PBT:**

Not applicable.

**vPvB:**

Not applicable.

**Other adverse effects**

No further relevant information available.

Toxicity											
Aquatic toxicity:	No further relevant information available.										
Persistence and degradability:	No further relevant information available.										
Behavior in environmental systems:											
Bioaccumulative potential:	No further relevant information available.										
Mobility in soil:	No further relevant information available.										
Additional ecological information:											
General notes:											
Water hazard class 2 (Self-assessment):	hazardous for water										
Do not allow product to reach	ground water, water course or sewage system.										
										(Contd. on page 8)	
											US

**SECTION 13: Disposal considerations****Waste treatment methods****Recommendation**

Must not be disposed of together with household garbage. Do not allow product to reach sewage system.

**Uncleaned packagings**

**Recommendation**

Disposal must be made according to official regulations.

**Recommended cleansing agent**

Water, if necessary with cleansing agents.

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**SECTION 14: Transport information****UN-Number**

DOT, IMDG, IATA UN1648

**UN proper shipping name**

DOT, IATA Acetonitrile solution

IMDG ACETONITRILE solution

**Transport hazard class(es)****DOT**

Class: 3 Flammable liquids

Label: 3

**IMDG, IATA**

Class: 3 Flammable liquids

Label: 3

**Packing group**

DOT, IMDG, IATA II

**Environmental hazards**

Not applicable.

**Special precautions for user**

Warning: Flammable liquids

**Hazard identification number (Kemler code)**

33

**EMS Number**

F-E,S-D

**Stowage Category**

B

**Stowage Code**

SW2 Clear of living quarters.

## Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code

Not applicable.

## Transport/Additional information

### DOT:

### Quantity limitations

On passenger aircraft/rail: 5 L

On cargo aircraft only: 60 L

### IMDG:

### Limited quantities (LQ)

1L

### Excepted quantities (EQ)

Code: E2

Maximum net quantity per inner packaging: 30 ml

Maximum net quantity per outer packaging: 500 ml

### IATA:

### Remarks

When sold in quantities of less than or equal to 1 mL, or 1 g, with an Excepted Quantity Code of

E1, E2, E4, or E5, this item meets the De Minimis

Quantities exemption, per IATA 2.6.10.

Therefore packaging does not have to be labeled as

Dangerous Goods/Excepted Quantity.

### UN "Model Regulation"

UN 1648 ACETONITRILE SOLUTION, 3, II

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## SECTION 15: Regulatory information

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

No further relevant information available.

### Sara

Section 355 (extremely hazardous substances):	None of the ingredients is listed.
Section 313 (Specific toxic chemical listings):	75-05-8 Acetonitrile
TSCA (Toxic Substances Control Act):	75-05-8 Acetonitrile ACTIVE
Hazardous Air Pollutants 75-05-8 Acetonitrile	

### Proposition 65

Chemicals known to cause cancer:	None of the ingredients is listed.
Chemicals known to cause reproductive toxicity for females:	None of the ingredients is listed.
Chemicals known to cause reproductive toxicity for males:	None of the ingredients is listed.
Chemicals known to cause developmental toxicity:	None of the ingredients is listed.

### Carcinogenic categories

EPA (Environmental Protection Agency):

#### 75-05-8

Acetonitrile CBD, D

### TLV (Threshold Limit Value)

#### 75-05-8

Acetonitrile A4

### NIOSH-Ca (National Institute for Occupational Safety and Health)

None of the ingredients is listed.

### Chemical safety assessment

A Chemical Safety Assessment has not been carried out.

## SECTION 16: Other information

### Abbreviations and acronyms

IMDG: International Maritime Code for Dangerous Goods

DOT: US Department of Transportation

IATA: International Air Transport Association

EINECS: European Inventory of Existing Commercial Chemical Substances

ELINCS: European List of Notified Chemical Substances

CAS: Chemical Abstracts Service (division of the American Chemical Society)

NFPA: National Fire Protection Association (USA)

HMS: Hazardous Materials Identification System (USA)

VOC: Volatile Organic Compounds (USA, EU)

LC50: Lethal concentration, 50 percent

LD50: Lethal dose, 50 percent

PBT: Persistent, Bioaccumulative and Toxic vPvB: very Persistent and very Bioaccumulative

NIOSH: National Institute for Occupational Safety

OSHA: Occupational Safety & Health

TLV: Threshold Limit Value

PEL: Permissible Exposure Limit

REL: Recommended Exposure Limit

Flammable Liquids 2: Flammable liquids – Category 2

Acute Toxicity - Oral 4: Acute toxicity – Category 4

Eye Irritation 2A: Serious eye damage/eye irritation – Category 2A

**Disclaimer:**

The information in this MSDS is only applicable to the specified product, unless otherwise specified, it is not applicable to the mixture of this product and other substances. This MSDS only provides information on the safety of the product for those who have received the appropriate professional training for the user of the product. Users of this MSDS must make independent judgments on the applicability of this SDS. The authors of this MSDS will not be held responsible for any harm caused by the use of this MSDS.