

Chemical Safety Data Sheet MSDS / SDS

2-[(1R,6R)-3-methyl-6-prop-1-en-2-ylcyclohex-2-en-1-yl]-5-pentylbenzene-1,3-diol

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

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

Product name : 2-[(1R,6R)-3-methyl-6-prop-1-en-2-ylcyclohex-2-en-1-yl]-5-pentylbenzene-1,3-diol
CBnumber : CB93809366
CAS : 3556-78-3
Synonyms : 2-[(1R,6R)-3-Methyl-6-prop-1-en-2-ylcyclohex-2-en-1-yl]-5-pentylbenzene-1,3-diol

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

No data available

Hazard statements

No data available

SECTION 3: Composition/information on ingredients**Substance**

Product name : 2-[(1R,6R)-3-methyl-6-prop-1-en-2-ylcyclohex-2-en-1-yl]-5-pentylbenzene-1,3-diol
Synonyms : 2-[(1R,6R)-3-Methyl-6-prop-1-en-2-ylcyclohex-2-en-1-yl]-5-pentylbenzene-1,3-diol

CAS : 3556-78-3
MF : C21H30O2
MW : 314.46

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

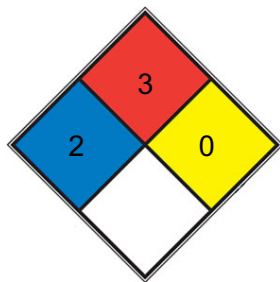
No further relevant information available.

SECTION 5: Firefighting measures

FIRE-FIGHTING MEASURES

Fire-fighting measure	Details
Suitable extinguishing agents	CO2, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.
Special hazards arising from the substance or mixture	Can release vapors that form explosive mixtures at temperatures at or above the flashpoint. Container explosion may occur under fire conditions. Emits toxic fumes under fire conditions. Sensitive to static discharge. Vapors can travel to a source of ignition and flash back.

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, [N₂](#))

SPEC.

HAZ.

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 section 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

PAC-3

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

Keep away from heat, sparks and flame.

Keep container tightly closed.

Store in accordance with information listed on the product insert.

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.

SECTION 8: Exposure controls/personal protection

Additional information about design of technical systems

No further data; see section 7.

Control parameters

Components with limit values that require monitoring at the workplace:

75-05-8 Acetonitrile	
PEL	Long-term value: 70 mg/m ³ , 40 ppm
REL	Long-term value: 34 mg/m ³ , 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

SECTION 9: Physical and chemical properties

Information on basic physicochemical properties

Appearance

Physical State

Liquid

Color

According to product specification

Odor

Characteristic

Structural Formula

C₂₁H₃₀O₂

Molecular Weight

314.5 g/mol

Odor Threshold

Not determined.

Formulation

A 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

2 °C (35.6 °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)

98.64 hPa (74 mm Hg)

Vapor Pressure at 50 °C (122 °F)

330 hPa (247.5 mm Hg)

Density at 20 °C (68 °F)

0.7822 g/cm³ (6.52746 lbs/gal)

Relative Density

1.025±0.06 g/cm³(Predicted)

Vapor Density

Not determined.

Evaporation Rate

Not determined.

Solubility in / Miscibility with

Acetonitrile: 50 mg/ml

Water at 25 °C (77 °F)

1000 g/l

Partition coefficient (n-octanol/water)

Not determined.

Viscosity**Dynamic**

at 20 °C (68 °F): 0.39 mPas

Kinematic

Not determined.

SOLUBILITY

Acetonitrile: 50 mg/ml

VOC content

0.00 % 0.0 g/l / 0.00 lb/gal

Solids content

0.0 %

Other information

No information available

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.

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	649 mg/kg (mouse)
ATE (Acute Toxicity Estimate)	Dermal	LD50	1,579 mg/kg (rabbit)
ATE (Acute Toxicity Estimate)	Inhalative	LC50/4 h	11.6 mg/l

75-05-8 Acetonitrile	Oral	LD50	617 mg/kg (mouse) (OECD Test Guideline 401)
75-05-8 Acetonitrile	Dermal	LD50	1,500 mg/kg (rabbit) (Expert Judgement) Remarks: Classified according to Regulation (EU) 1272/2008, Annex VI (Table 3.1/3.2)
75-05-8 Acetonitrile	Inhalative	LC50/4 h	6.022 mg/l (mouse) (OECD Test Guideline 403)

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

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.

Danger to drinking water if even small quantities leak into the ground.

Results of PBT and vPvB assessment

PBT

Not applicable.

vPvB

Not applicable.

PBT:

Not applicable.

vPvB:

Not applicable.

Other adverse effects

No further relevant information available.

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.

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

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):
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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

ATA: 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.