ChemicalBook

Chemical Safety Data Sheet MSDS / SDS

1,3-DIDECYL-5-[3-(1,3-DIDECYLHEXAHYDRO-4,6-DIOXO-2-THIOXO-5-PYRIMIDINYL)-2-PROPENYLIDENE]DIHYDRO-2-THIOXO-4,6-(1H,5H)-PYRIMIDINEDIONE

Revision Date:2026-03-20 Revision Number:1

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

Product identifier

Product name	: 1,3-DIDECYL-5-[3-(1,3-DIDECYLHEXAHYDRO-4,6-DIOXO-2-THIOXO-5-PYRIMIDINYL)-2-PROPENYLIDENE]DIHYDRO-2-THIOXO-4,6-(1H,5H)-PYRIMIDINEDIONE
CBnumber	: CB3171336
CAS	: 169211-45-4
Synonyms	: DISBAC10;1,3-didecyl-5-[(E)-3-(1,3-didecyl-4,6-dioxo-2-sulfanylidene-1,3-diazinan-5-yl)prop-2-enylidene]-2-sulfanylidene-1,3-diazinane-4,6-dione

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

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

P405 Store locked up.

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

P403+P233 Store in a well-ventilated place. Keep container tightly closed.

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

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

P312 Call a POISON CENTER or doctor/physician if you feel unwell.

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

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

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

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

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

P264 Wash skin thouroughly after handling.

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

P243 Take precautionary measures against static discharge.

P242 Use only non-sparking tools.

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

P240 Ground/bond container and receiving equipment.

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

Hazard statements

H336 May cause drowsiness or dizziness

H319 Causes serious eye irritation

H225 Highly Flammable liquid and vapour

SECTION 3: Composition/information on ingredients

Substance

Product name	: 1,3-DIDECYL-5-[3-(1,3-DIDECYLHEXAHYDRO-4,6-DIOXO-2-THIOXO-5-PYRIMIDINYL)-2-PROPENYLIDENE]DIHYDRO-2-THIOXO-4,6-(1H,5H)-PYRIMIDINEDIONE
Synonyms	: DISBAC10;1,3-didecyl-5-[(E)-3-(1,3-didecyl-4,6-dioxo-2-sulfanylidene-1,3-diazinan-5-yl)prop-2-enylidene]-2-sulfanylidene-1,3-diazinane-4,6-dione
CAS	: 169211-45-4
MF	: C51H88N4O4S2
MW	: 885.4

SECTION 4: First aid measures

Description of first aid measures

General information

Immediately remove any clothing soiled by the product.

After inhalation

Supply fresh air; consult doctor in case of complaints.

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

If symptoms persist consult 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

Extinguishing media

Suitable extinguishing agents

CO_2, extinguishing powder or water spray. Fight larger fires with water spray or alcohol resistant foam.

For safety reasons unsuitable extinguishing agents

Water with full jet

Special hazards arising from the substance or mixture

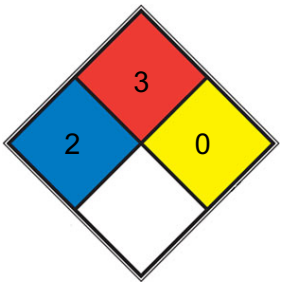
No further relevant information available.

Advice for firefighters

Protective equipment

No special measures required.

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

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

79-20-9 Methyl acetate 250 ppm

PAC-2

79-20-9 Methyl acetate 1,700 ppm

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

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 item 7.

Control parameters

Components with limit values that require monitoring at the workplace:

79-20-9 Methyl acetate	
PEL	Long-term value: 610 mg/m³, 200 ppm
REL	Short-term value: 760 mg/m³, 250 ppm Long-term value: 610 mg/m³, 200 ppm
TLV	Short-term value: 250 ppm Long-term value: 200 ppm

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

Fluid

Color

Colorless

Odor

Pleasant

Structural Formula

C51H88N4O4S2

Molecular Weight

885.4 g/mol

Odor Threshold

Not determined.

pH

Not determined.

Change in condition

Melting point/Melting range

-98.05 °C (-144.5 °F)

Boiling point/Boiling range

57 °C (134.6 °F)

Flash point

-13 °C (8.6 °F)

Flammability (solid,gas)

Highly flammable.

Ignition temperature

455 °C (851 °F)

Decomposition temperature

Not determined.

Auto igniting

Product is not selfigniting.

Danger of explosion

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

Explosion limits

Lower: 3.1 Vol %

Upper: 16 Vol %

Vapor Pressure at 20 °C (68 °F)

220 hPa (165 mm Hg)

Density at 20 °C (68 °F)

0.93 g/cm³ (7.76085 lbs/gal)

Relative Density

1.07±0.1 g/cm3(Predicted)

Vapor Density

Not determined.

Evaporation Rate

Not determined.

Solubility in / Miscibility with

Water at 20 °C (68 °F)

330 g/l

Partition coefficient (n-octanol/water)

Not determined.

Viscosity

Dynamic

Not determined.

Kinematic

Not determined.

Organic solvents

99.0 %

VOC content

0.00 % 0.0 g/l / 0.00 lb/gal

Solids content

1.0 %

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
79-20-9 Methyl acetate	Oral	LD50	>5,000 mg/kg (rat) 3,705 mg/kg (rabbit)
79-20-9 Methyl acetate	Dermal	LD50	>5,000 mg/kg (rabbit) Inhalative TCLO 15,000 mg/m³ (hmn) Irritation of skin Irritation 500 mg/24h (rabbit) Irritation 40 mg/kg/24h (rabbit) Irritation of eyes Irritation 100 mg/24h (rabbit)
79-20-9 Methyl acetate	Intraperitoneal	LD50	70 mg/kg (mouse)

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

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 1 (Self-assessment) slightly hazardous for water

Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.

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.

SECTION 14: Transport information

UN-Number

DOT, IMDG, IATA UN1231

UN proper shipping name

DOT, IATA Methyl acetate

IMDG METHYL ACETATE

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

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 1231 METHYL ACETATE, 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):	None of the ingredients is listed.
TSCA (Toxic Substances Control Act):	79-20-9 Methyl acetate ACTIVE
Hazardous Air Pollutants:	None of the ingredients is listed.

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):	None of the ingredients is listed.

TLV (Threshold Limit Value)

None of the ingredients is listed.

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)

HMIS: 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

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

Specific Target Organ Toxicity - Single Exposure 3: Specific target organ toxicity (single exposure) – Category 3