

Material Safety Data Sheet

2,2'-[[6,6,12,12-tetrakis(4-hexylphenyl)-s-indacenodithieno[3,2-b]

thiophene]methylidyne(3-oxo-1H-indene-2,1(3H)-diylidene)]]bis(propanedinitrile)

Section 1 - Chemical Product and Company Identification

MSDSName:

2,2'-[[6,6,12,12-tetrakis(4-hexylphenyl)-s-indacenodithieno[3,2-b]thiophene]methylidyne(3-oxo-1H-indene-2,1(3H)-diylidene)]]bis(propanedinitrile)

Catalog Numbers: S6655

Synonyms:

Company Identification:

Derthon Optoelectronic Materials Sci. Tech. Co., Ltd.
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Section 2 - Composition, Information on Ingredients

CAS RN [1664293-06-4]

Chemical Name:

2,2'-[[6,6,12,12-tetrakis(4-hexylphenyl)-s-indacenodithieno[3,2-b]thiophene]methylidyne(3-oxo-1H-indene-2,1(3H)-diylidene)]]bis(propanedinitrile)

Formula: C₉₄H₈₂N₄O₂S₄

Purity: >99%

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Appearance: Solid

Caution! May cause eye and skin irritation. May cause respiratory and digestive tract irritation. The toxicological properties of this material have not been fully investigated.

Target Organs: No data found.

Potential Health Effects

Eye: May cause eye irritation.

Skin: May cause skin irritation.

Ingestion: May cause irritation of the digestive tract. The toxicological properties of this substance have not been fully investigated.

Inhalation: May cause respiratory tract irritation. The toxicological properties of this substance have not been fully investigated.

Chronic: No information found.

Section 4 - First Aid Measures

Eyes: Flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical aid.

Skin: Get medical aid. Flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes. Wash clothing before reuse.

Ingestion: Never give anything by mouth to an unconscious person. Get medical aid. Do NOT induce vomiting. If conscious and alert, rinse mouth and drink 2-4 cupfuls of milk or water.

Inhalation: Remove from exposure and move to fresh air immediately. If not breathing, give artificial respiration. If breathing is difficult, give oxygen. Get medical aid.

Notes to Physician: Treat symptomatically and supportively.

Section 5 - Fire Fighting Measures

General Information: As in any fire, wear a self-contained breathing apparatus in pressure-demand, MSHA/NIOSH (approved or equivalent), and full protective gear.

During a fire, irritating and highly toxic gases may be generated by thermal decomposition or combustion. Runoff from fire control or dilution water may cause pollution.

Extinguishing Media: Use agent most appropriate to extinguish fire.

Flash Point: Not available.

Autoignition Temperature: Not available.

Explosion Limits, Lower: Not available.

Upper: Not available.

NFPA Rating: (estimated) Health: 1; Flammability: 0; Instability: 0

Section 6 - Accidental Release Measures

General Information: Use proper personal protective equipment as indicated in Section 8.

Spills/Leaks: Vacuum or sweep up material and place into a suitable disposal container. Clean up spills immediately, observing precautions in the Protective Equipment section. Avoid generating dusty conditions. Provide ventilation.

Section 7 - Handling and Storage

Handling: Wash thoroughly after handling. Remove contaminated clothing and wash before reuse. Use with adequate ventilation. Minimize dust generation and accumulation. Avoid contact with eyes, skin, and clothing. Keep container tightly closed. Avoid ingestion and inhalation.

Storage: Store in a tightly closed container. Store in a cool, dry, well-ventilated area away from incompatible substances.

Section 8 - Exposure Controls, Personal Protection

Engineering Controls: Facilities storing or utilizing this material should be equipped with an eyewash facility and a safety shower. Use process enclosure, local exhaust ventilation, or other engineering controls to control airborne levels.

OSHA Vacated PELs: CAS:1664293-06-4: No OSHA Vacated PELs are listed for this chemical.

Personal Protective Equipment

Eyes: Wear chemical splash goggles. Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin: Wear appropriate protective gloves to prevent skin exposure.

Clothing: Wear appropriate protective clothing to minimize contact with skin.

Respirators: Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Section 9 - Physical and Chemical Properties

Physical State: Solid

Appearance: Blue-Black

Odor: Not available.

PH: Not available.

Vapor Pressure: Not available.

Vapor Density: Not available.

Evaporation Rate: Not available.

Viscosity: Not available.

Boiling Point: Not available.

Freezing/Melting Point: Not available.

Decomposition Temperature: Not available.

Solubility: Insoluble in water.

Specific Gravity/Density: Not available.

Molecular Formula: $C_{94}H_{82}N_4O_2S_4$

Molecular Weight: 1427.94

HOMO/LUMO: HOMO = -5.48 eV, LUMO = -3.83 eV

Section 10 - Stability and Reactivity

Chemical Stability: Stable under normal temperatures and pressures.

Conditions to Avoid: Incompatible materials, dust generation, excess heat, strong oxidants.

Incompatibilities with Other Materials: Oxidizing agents.

Hazardous Decomposition Products: nitrogen oxides, carbon monoxide, stannic oxide, sulfur oxides, irritating and toxic fumes and gases, carbon dioxide.

Hazardous Polymerization: Has not been reported

Section 11 - Toxicological Information

RTECS#:

CAS# [1664293-06-4]

LD50/LC50:

Not available.

Carcinogenicity:

CAS# [1664293-06-4]: Not listed by ACGIH, IARC, NTP, or CA Prop 65.

Epidemiology: No information found

Teratogenicity: No information found

Reproductive Effects: No information found

Mutagenicity: No information found

Neurotoxicity: No information found

Other Studies:

Section 12 - Ecological Information

No information available.

Section 13 - Disposal Considerations

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. US EPA guidelines for the classification determination are listed in 40 CFR Parts 261.3. Additionally, waste generators must consult state and local hazardous waste regulations to ensure complete and accurate classification.

RCRA P-Series: None listed.

RCRA U-Series: None listed.

Section 14 - Regulatory Information

US FEDERAL

TSCA

CAS# [1664293-06-4] is not listed on the TSCA inventory. It is for research and development use only.

Health & Safety Reporting List

None of the chemicals are on the Health & Safety Reporting List.

Chemical Test Rules

None of the chemicals in this product are under a Chemical Test Rule.

Section 12b

None of the chemicals are listed under TSCA Section 12b.

TSCA Significant New Use Rule

None of the chemicals in this material have a SNUR under TSCA.

CERCLA Hazardous Substances and corresponding RQs

None of the chemicals in this material have an RQ.

SARA Section 302 Extremely Hazardous Substances

None of the chemicals in this product have a TPQ.

Section 313 No chemicals are reportable under Section 313.

Clean Air Act:

This material does not contain any hazardous air pollutants.

This material does not contain any Class 1 Ozone depleters.

This material does not contain any Class 2 Ozone depleters.

Clean Water Act:

None of the chemicals in this product are listed as Hazardous Substances under the CWA.

None of the chemicals in this product are listed as Priority Pollutants under the CWA.

None of the chemicals in this product are listed as Toxic Pollutants under the CWA.

OSHA:

None of the chemicals in this product are considered highly hazardous by OSHA.

STATE

CAS# [1664293-06-4] is not present on state lists from CA, PA, MN, MA, FL, or NJ.

California Prop 65

California No Significant Risk Level: None of the chemicals in this product are listed.

European/International Regulations

European Labeling in Accordance with EC Directives

Hazard Symbols:

Not available.

Risk Phrases:

Safety Phrases:

S 24/25 Avoid contact with skin and eyes.

WGK (Water Danger/Protection)

CAS# [1664293-06-4]: No information available.

Canada - DSL/NDSL

CAS# [1664293-06-4] is listed on the DSL or NDSL list.

Canada - WHMIS

WHMIS: Not available.

This product has been classified in accordance with the hazard criteria of the Controlled Products Regulations and the MSDS contains all of the information required by those regulations.

Canadian Ingredient Disclosure List

Section 15- ICAO/IATA Transport Information

With regard to Transport, the following regulations are cited and considered.

The International Civil Aviation Organization (ICAO) Technical Instructions (2017-2018 Edition)

This chemical is no dangerous goods, no hazard Class, no UN Number

Not regulated as a hazardous material on US Department of Transport (DOT) 49 code of Federal regulations.

Environment hazards

ADR/RID: No

IATA_DGR: No

IMDG Marine Pollutant: No

Packing:

Each packaging is complete and seal, without no damage. In the process of transportation to prevent sun, rain, heat.

Section 16 - Additional Information

The information above is believed to be accurate and represents the best information currently available to us. However, we make no warranty of merchantability or any other warranty, express or implied, with respect to such information, and we assume no liability resulting from its use. Users should make their own investigations to determine the suitability of the information for their particular purposes. In no event shall Derthon Optoelectronic Materials Sci. Tech. Co., Ltd. Be liable for any claims, losses, or damages of any third party or for lost profits or any special, indirect, incidental, consequential or exemplary damages, howsoever arising, even if Derthon Optoelectronic Materials Sci. Tech. Co., Ltd has been advised of the possibility of such damages.