

SAFETY DATA SHEET

Creation Date 10-Feb-2011

Revision Date 19-Dec-2025

Revision Number 6

This safety data sheet was created pursuant to the requirements of: US OSHA Hazard Communication Standard 2024 (29 CFR 1910.1200)

1. Identification

| | |
|---------------------|---|
| Product Name | 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate |
| Cat No. : | AC422000000; AC422000010; AC422000050 |
| CAS No | 6846-50-0 |
| Synonyms | Kodaflex TXIB |

Recommended Use
Uses advised against

Laboratory chemicals.
Food, drug, pesticide or biocidal product use.

Details of the supplier of the safety data sheet

Company

Fisher Scientific Company
One Reagent Lane
Fair Lawn, NJ 07410
Tel: (201) 796-7100

Acros Organics
One Reagent Lane
Fair Lawn, NJ 07410

Emergency Telephone Number

For information **US** call: 001-800-227-6701 / **Europe** call: +32 14 57 52 11
Emergency Number **US**:001-201-796-7100 / **Europe**: +32 14 57 52 99
CHEMTREC Tel. No. **US**:001-800-424-9300 / **Europe**:001-703-527-3887

2. Hazard(s) identification

Classification

Classification according to [US] OSHA (29 CFR 1910.1200, 2024)

Label Elements

None required

Hazards not otherwise classified (HNOC)

Harmful to aquatic life with long lasting effects

Hazards classified under paragraph (d)(1)(ii) of 1910.1200

No information available

3. Composition/information on Ingredients

| Component | CAS No | Weight % |
|---|-----------|----------|
| 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate | 6846-50-0 | >95 |

4. First-aid measures

| | |
|--|--|
| Eye Contact | Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Get medical attention. |
| Skin Contact | Wash off immediately with soap and plenty of water while removing all contaminated clothes and shoes. Get medical attention. |
| Inhalation | Remove from exposure, lie down. Remove to fresh air. If not breathing, give artificial respiration. Get medical attention. |
| Ingestion | Clean mouth with water. Get medical attention. |
| Most important symptoms and effects | No information available. |
| Notes to Physician | Treat symptomatically |

5. Fire-fighting measures

| | |
|---|--|
| Suitable Extinguishing Media | Water spray. Carbon dioxide (CO ₂). Dry chemical. Chemical foam. |
| Unsuitable Extinguishing Media | No information available |
| Flash Point | 128 °C / 262.4 °F |
| Method - | No information available |
| Autoignition Temperature | 423 °C / 793.4 °F |
| Explosion Limits | |
| Upper | No data available |
| Lower | No data available |
| Sensitivity to Mechanical Impact | No information available |
| Sensitivity to Static Discharge | No information available |

Specific Hazards Arising from the Chemical

Keep product and empty container away from heat and sources of ignition.

Hazardous Combustion Products

Carbon monoxide (CO). Carbon dioxide (CO₂).

Protective Equipment and Precautions for Firefighters

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

NFPA

| Health | Flammability | Instability | Physical hazards |
|--------|--------------|-------------|------------------|
| 0 | 1 | 0 | N/A |

6. Accidental release measures

Personal Precautions Ensure adequate ventilation. Use personal protective equipment as required.
Environmental Precautions See Section 12 for additional Ecological Information. Avoid release to the environment. Collect spillage. Do not flush into surface water or sanitary sewer system.

Methods for Containment and Clean Up Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust). Keep in suitable, closed containers for disposal.

7. Handling and Storage

Handling Avoid contact with skin and eyes. Do not breathe mist/vapors/spray.

Storage. Keep in a dry, cool and well-ventilated place. Keep container tightly closed. Incompatible Materials. Strong oxidizing agents.

8. Exposure controls / personal protection

Exposure Guidelines This product does not contain any hazardous materials with occupational exposure limits established by the region specific regulatory bodies.

Engineering Measures None under normal use conditions.

Personal Protective Equipment

Eye/face Protection 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 and body protection Wear appropriate protective gloves and clothing to prevent skin exposure.

Respiratory Protection No protective equipment is needed under normal use conditions.

Recommended Filter type: Particle filter.

Hygiene Measures Handle in accordance with good industrial hygiene and safety practice.

9. Physical and chemical properties

Appearance

Physical State Liquid

Color Colorless

Odor No information available

Odor Threshold No information available

Property

Melting Point/Range -70 °C / -94 °F

Softening Point No data available

Boiling Point/Range 280 °C / 536 °F

Flash Point 128 °C / 262.4 °F

Flammability (liquid) No data available

Flammability (solid,gas) Not applicable

Explosion Limits No data available

Values

Remarks

Method

Autoignition Temperature 423 °C / 793.4 °F

Decomposition Temperature No data available

pH No information available

Viscosity No data available

Water Solubility Insoluble in water

Solubility in other solvents No information available

@ 760 mmHg

Method - No information available

Liquid

Partition Coefficient (n-octanol/water)

| | |
|-----------------------------------|-------------------------|
| Vapor Pressure | No data available |
| Density / Specific Gravity | 0.940 |
| Bulk Density | Not applicable |
| Vapor Density | 9.9 (Air = 1.0) |
| Particle characteristics | (liquid) Not applicable |

Other Information

| | |
|--------------------------|------------|
| Molecular Formula | C16 H30 O4 |
| Molecular Weight | 286.4 |

10. Stability and reactivity

Reactive Hazard None known, based on information available

Stability Stable under normal conditions.

Conditions to Avoid Incompatible products.

Incompatible Materials Strong oxidizing agents

Hazardous Decomposition Products Carbon monoxide (CO), Carbon dioxide (CO₂)

Hazardous Polymerization Hazardous polymerization does not occur.

Hazardous Reactions None under normal processing.

11. Toxicological information**Information on expected route of exposure**

Inhalation Not an expected route of exposure.

Ingestion No known effect based on information supplied.

Eyes Not an expected route of exposure.

Skin No known effect based on information supplied.

Toxicology data for the components

| Component | LD50 Oral | LD50 Dermal | LC50 Inhalation |
|---|---------------------------|------------------------------|-----------------------------|
| 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate | LD50 > 3200 mg/kg (Rat) | LD50 > 2000 mg/kg (Rabbit) | LC50 > 5.3 mg/L (Rat) 6 h |

Toxicologically Synergistic Products No information available

(b) skin corrosion/irritation; No data available

(c) serious eye damage/irritation; No data available

(d) respiratory or skin sensitization;

Respiratory No data available
Skin No data available

(e) germ cell mutagenicity; No data available

(f) carcinogenicity;

The table below indicates whether each agency has listed any ingredient as a carcinogen

| Component | CAS No | IARC | NTP | ACGIH | OSHA | Mexico |
|---|-----------|------------|------------|------------|------------|------------|
| 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate | 6846-50-0 | Not listed |

(g) reproductive toxicity; No data available

(h) STOT-single exposure; No data available

(i) STOT-repeated exposure; No data available

Target Organs No information available.

(j) aspiration hazard; No data available

Symptoms / effects,both acute and delayed No information available.

Other Adverse Effects The toxicological properties have not been fully investigated.

Endocrine Disrupting Properties This product does not contain any known or suspected endocrine disruptors.

12. Ecological information

Ecotoxicity

The product contains following substances which are hazardous for the environment. Toxic to aquatic organisms, may cause long-term adverse effects in the aquatic environment.

| Component | Freshwater Algae | Freshwater Fish | Microtox | Water Flea |
|--|------------------|---|------------|----------------------|
| 2,2,4-Trimethyl-1,3-pentane diol diisobutyrate | Not listed | LC50: > 1.55 mg/L, 96h static (Pimephales promelas) | Not listed | EC5 = 1.46 mg/L, 48h |

Persistence and Degradability Insoluble in water Persistence is unlikely based on information available.

Bioaccumulation/ Accumulation No information available.

Mobility No information available.

13. Disposal considerations

Waste Disposal Methods Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations to ensure complete and accurate classification.

14. Transport information

DOT Not regulated

TDG Not regulated

IATA Not regulated

IMDG/IMO Not regulated

15. Regulatory Information

United States of America Inventory

| Component | CAS No | TSCA | TSCA Inventory notification - Active-Inactive | TSCA - EPA Regulatory Flags |
|---|-----------|------|---|-----------------------------|
| 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate | 6846-50-0 | X | ACTIVE | - |

Legend:

TSCA US EPA (TSCA) - Toxic Substances Control Act, (40 CFR Part 710)

X - Listed

'-' - Not Listed

TSCA - Per 40 CFR 751, Regulation of Certain Chemical Substances & Mixtures, Under TSCA Section 6(h) (PBT) Not applicable

TSCA 12(b) - Notices of Export Not applicable

International Inventories

Canada (DSL/NDSL), Europe (EINECS/ELINCS/NLP), Philippines (PICCS), Japan (ENCS), Japan (ISHL), Australia (AICS), China (IECSC), Korea (KECL).

| Component | CAS No | DSL | NDSL | EINECS | PICCS | ENCS | ISHL | AICS | IECSC | KECL |
|---|-----------|-----|------|-----------|-------|------|------|------|-------|----------|
| 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate | 6846-50-0 | X | - | 229-934-9 | X | X | X | X | X | KE-24877 |

KECL - NIER number or KE number (<http://ncis.nier.go.kr/en/main.do>)

U.S. Federal Regulations**SARA 313**

Section 313 of Title III of the Superfund Amendments and Reauthorization Act of 1986 (SARA). This product does not contain any chemicals which are subject to the reporting requirements of the Act and Title 40 of the Code of Federal Regulations, Part 372

SARA 311/312 Hazard Categories

Should this product meet EPCRA 311/312 Tier reporting criteria at 40 CFR 370, refer to Section 2 of this SDS for appropriate classifications.

CWA (Clean Water Act) Not applicable

Clean Air Act Not applicable

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA

This material, as supplied, does not contain any substances regulated as hazardous substances under the Comprehensive Environmental Response Compensation and Liability Act (CERCLA) (40 CFR 302) or the Superfund Amendments and Reauthorization Act (SARA) (40 CFR 355). There may be specific reporting requirements at the local, regional, or state level pertaining to releases of this material.

California Proposition 65 This product does not contain any Proposition 65 chemicals.

U.S. State Right-to-Know Regulations Not applicable

U.S. Department of Transportation

Reportable Quantity (RQ): N
DOT Marine Pollutant N
DOT Severe Marine Pollutant N

U.S. Department of Homeland Security This product does not contain any DHS chemicals.

Other International Regulations

Mexico - Grade No information available

Authorisation/Restrictions according to EU REACH Not applicable

| Component | CAS No | REACH (1907/2006) - Annex XIV - Substances Subject to Authorization | REACH (1907/2006) - Annex XVII - Restrictions on Certain Dangerous Substances | REACH Regulation (EC 1907/2006) article 59 - Candidate List of Substances of Very High Concern (SVHC) |
|---|-----------|---|---|---|
| 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate | 6846-50-0 | - | - | - |

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

| Component | CAS No | OECD HPV | Persistent Organic Pollutant | Ozone Depletion Potential | Restriction of Hazardous Substances (RoHS) |
|---|-----------|----------|------------------------------|---------------------------|--|
| 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate | 6846-50-0 | Listed | Not applicable | Not applicable | Not applicable |

Contains component(s) that meet a 'definition' of per & poly fluoroalkyl substance (PFAS)?

Not applicable

Other International Regulations

| Component | CAS No | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Major Accident Notification | Seveso III Directive (2012/18/EC) - Qualifying Quantities for Safety Report Requirements | Rotterdam Convention (PIC) | Basel Convention (Hazardous Waste) |
|---|-----------|---|--|----------------------------|------------------------------------|
| 2,2,4-Trimethyl-1,3-pentanediol diisobutyrate | 6846-50-0 | Not applicable | Not applicable | Not applicable | Not applicable |

16. Other Information

Prepared By Product stewardship (Regulatory Affairs)
Thermo Fisher Scientific
email - begel.sdsdesk@thermofisher.com

Creation Date 10-Feb-2011
Revision Date 19-Dec-2025
Print Date 19-Dec-2025
Revision Summary Updated to the U.S. Department of Labor's Occupational Safety and Health Administration (OSHA) which published its Final Rule in the Federal Register revising the Hazard Communication Standard (HCS/HazCom), 29 CFR 1910.1200 (2024) (HCS §1910.1200, 2024), May 20, 2024, effective July 19, 2024.

Disclaimer

The information provided in this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guidance for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered a warranty or quality specification. The information

relates only to the specific material designated and may not be valid for such material used in combination with any other materials or in any process, unless specified in the text

End of SDS