

SAFETY DATA SHEET

Creation Date 10-Feb-2011

Revision Date 26-Dec-2021

Revision Number 5

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 Laboratory chemicals.
Uses advised against 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-ACROS-01 / **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 under 2012 OSHA Hazard Communication Standard (29 CFR 1910.1200)

Label Elements

None required

Hazards not otherwise classified (HNOC)

Harmful to aquatic life with long lasting effects

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
0

Flammability
1

Instability
0

Physical hazards
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 Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder,

Up 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 limitsestablished 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.

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

9. Physical and chemical properties

Physical State	Liquid
Appearance	Colorless
Odor	No information available
Odor Threshold	No information available
pH	No information available
Melting Point/Range	-70 °C / -94 °F
Boiling Point/Range	280 °C / 536 °F @ 760 mmHg
Flash Point	128 °C / 262.4 °F
Evaporation Rate	No information available
Flammability (solid,gas)	Not applicable
Flammability or explosive limits	
Upper	No data available
Lower	No data available
Vapor Pressure	No information available
Vapor Density	9.9 (Air = 1.0)
Specific Gravity	0.940
Solubility	No information available
Partition coefficient; n-octanol/water	No data available
Autoignition Temperature	423 °C / 793.4 °F
Decomposition Temperature	No information available
Viscosity	No information available
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 (CO ₂)
Hazardous Polymerization	Hazardous polymerization does not occur.
Hazardous Reactions	None under normal processing.

11. Toxicological information

Acute Toxicity

Product Information

Component Information

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

Delayed and immediate effects as well as chronic effects from short and long-term exposure

Irritation No information available

Sensitization No information available

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	Not listed	Not listed	Not listed	Not listed

Mutagenic Effects No information available

Reproductive Effects No information available.

Developmental Effects No information available.

Teratogenicity No information available.

STOT - single exposure None known

STOT - repeated exposure None known

Aspiration hazard No information available

Symptoms / effects, both acute and delayed No information available

Endocrine Disruptor Information No information available

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

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	Not listed	LC50: > 1.55 mg/L, 96h	Not listed	EC5 = 1.46 mg/L, 48h

diol diisobutyrate		static (Pimephales promelas)		
--------------------	--	------------------------------	--	--

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 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 Not applicable

SARA 311/312 Hazard Categories See section 2 for more information

CWA (Clean Water Act) Not applicable

Clean Air Act Not applicable

OSHA - Occupational Safety and Health Administration Not applicable

CERCLA Not applicable

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

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

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 Regulatory Affairs
Thermo Fisher Scientific
Email: EMSDS.RA@thermofisher.com

Creation Date 10-Feb-2011
Revision Date 26-Dec-2021
Print Date 26-Dec-2021
Revision Summary This document has been updated to comply with the US OSHA HazCom 2012 Standard replacing the current legislation under 29 CFR 1910.1200 to align with the Globally Harmonized System of Classification and Labeling of Chemicals (GHS).

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