Safety Data Sheet

5,6-Dimethylxantheonone-4-acetic acid

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*Prepared in accordance with EU REACH Regulation (REACH 1907/2006 with amendment 2020/878)

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

1.1 Product identifier

Product Name	5,6-Dimethylxantheonone-4-acetic acid
Product Model	98%
Cat No.	A011843
Synonyms	Vadimezan; DMXAA; ASA-404
CAS No.	117570-53-3
EC No.	700-141-4
Molecular Formula	$C_{17}H_{14}O_4$
REACH Registration Number	Not available from the supplier. The applicability of REACH registration obligations shall be assessed by the EU importer based on the actual annual import tonnage, use and applicable exemptions.
UFI	Not applicable

1.2 Relevant identified uses of the substance or mixture and uses advised against

Relevant identified uses	Laboratory chemicals / R&D use only
Uses advised against	Food, drug, cosmetic, household or other uses

1.3 Details of the supplier of the Safety Data Sheet

Supplier Name	Pharmate GmbH
Supplier Address	Monschauer Str. 12, Düsseldorf, Germany
Supplier Post Code	40549
Supplier Telephone	+49 211 54224195
Supplier Fax	——
Supplier E-mail	info@pharmaten.de
Manufacturer Name	Anhui Senrise Technology Co., Ltd.
Manufacturer Address	No. 88, Weisan Road, High-tech Development Zone, Daguan District, Anqing, Anhui Province, China
Manufacturer Post Code	246005
Manufacturer Telephone	400-005-6266
Manufacturer Fax	+86（0）556-5555368
Manufacturer E-mail	Service@3ASenrise.com

1.4 Emergency telephone number

Emergency telephone number	0800 181 7059 (CHEMTREC Germany) Additional numbers: +44 20 3885 0382 / +1 703 527 3887 CHEMTREC Customer Number (CCN): 1025941

Opening hours	24h

Part 2: Hazards identification

2.1 CLP classification according to Regulation (EC) No. 1272/2008 with amendment 2023/707

Acute Toxicity - Oral	Category 4
Hazardous to the aquatic environment - short-term (acute) hazard	Category 1

2.2 Label elements

Hazard pictograms	
Signal word	**Warning**

Hazard statements

H302	Harmful if swallowed
H400	Very toxic to aquatic life

Precautionary statements

◆Prevention

P264	Wash hands and other parts of the body (if related) thoroughly after handling.
P270	Do not eat, drink or smoke when using this product.
P273	Avoid release to the environment.

◆Response

P330	Rinse mouth.
P391	Collect spillage.
P301+P312	IF SWALLOWED: Call a POISON CENTER/ doctor, if you feel unwell.

◆Storage

Storage	Not applicable

◆Disposal

P501	Dispose of contents/container in accordance with local/regional/national/ international regulations.

2.3 Other hazards

◆Results of PBT and vPvB assessment

Component	Results of PBT and vPvB assessment [according to (EC) No 1907/2006 with amendment 2020/878]
5,6-Dimethylxantheonone-4-acetic acid	No information available

◆Results of endocrine disrupting properties assessment

Component	Results of endocrine disrupting properties assessment [according to (EU) No 2017/2100 or (EU) No 2018/605]

	Human endocrine disruptor	Environmental endocrine disruptor
5,6-Dimethylxantheonone-4-acetic acid	No information available	No information available

◆Other

	Not applicable.

Part 3: Composition/information on ingredients

3.1 Substance

Component	Weight % content(or range)	Classification according to Regulation (EC) No. 1272/2008 with amendment 2023/707 [CLP]	SCL, M-factor and ATE
5,6-Dimethylxantheonone-4-acetic acid CAS No.：117570-53-3 EC No.：700-141-4 Index No.：-	≥ 98	Acute Toxicity - Oral, Category 4, H302; Hazardous to the aquatic environment - short-term (acute) hazard, Category 1, H400	-

3.2 Mixture

	Not applicable

Part 4: First aid measures

4.1 Description of first aid measures

General advice	Immediate medical attention is required. Show this safety data sheet (SDS) to the doctor in attendance.
Eye contact	Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician if feel uncomfortable.
Skin contact	Take off contaminated clothing and shoes immediately. Wash off with plenty of soap and water for at least 15 minutes and consult a physician if feel uncomfortable.
Ingestion	Never give anything by mouth to an unconscious person. Call a physician or Poison Control Center immediately.
Inhalation	Move victim into fresh air. If breathing is difficult, give oxygen. Do not use mouth to mouth resuscitation if victim ingested or inhaled the substance. If not breathing, give artificial respiration and consult a physician immediately.
Protecting of first-aiders	Ensure that medical personnel are aware of the substance involved. Take precautions to protect themselves and prevent spread of contamination.

4.2 Most important symptoms/effects, acute and delayed

1	Substance accumulation, in the human body, may occur and may cause some concern following repeated or long-term occupational exposure.

4.3 Indication of any immediate medical attention and special treatment needed

1	Treat symptomatically.
2	Symptoms may be delayed.

Part 5: Fire-fighting measures

5.1 Extinguishing media

Suitable extinguishing media	Small fire: dry chemical, CO_2, water spray or regular foam; Large fire: water spray, fog or regular foam; Fire involving tanks: cool containers with flooding quantities of water until well after fire is out.

Unsuitable extinguishing media	Large fire: Do not scatter spilled material with high-pressure water streams.

5.2 Specific hazards arising from the substance or mixture

1	Development of hazardous combustion gases or vapor possible in the event of fire.
2	Exposure to heat or contact with flames may result in expansion or explosive decomposition.

5.3 Advice for firefighters

1	As in any fire, wear self-contained breathing apparatus (MSHA/NIOSH approved or equivalent) and full protective gear.
2	Fight fire from a safe distance, with adequate cover.
3	Prevent firefighting wastewater from contaminating surface water or the ground water system.

Part 6: Accidental release measures

6.1 Personal precautions, protective equipment and emergency procedures

1	Ensure adequate ventilation. Remove all sources of ignition. Take precautionary measures against static discharges.
2	Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.
3	Use personal protective equipment,do not breathe dust/fume.

6.2 Environmental precautions

1	Prevent further leakage or spillage if safe to do so.
2	Discharge into the environment must be avoided.

6.3 Methods and materials for containment and cleaning up

1	Keep leaks in a ventilated place.
2	Cut off the source of the leak as much as possible.
3	Adhered or collected material should be promptly disposed of, in accordance with appropriate laws and regulations.
4	Isolation of contaminated areas and restrictions on access.
5	It is recommended that emergency personnel wear dust masks.
6	Collect the spill with a clean shovel and place it in a clean, dry, loosely closed container and move the container away from the leak.

6.4 Reference to other sections

1	Personal Protective Equipment advice is contained in Section 8 of the SDS.
2	Disposal considerations advice is contained in Section 13 of the SDS.

Part 7: Handling and storage

7.1 Precautions for safe handling

◆ Protective measures

1	Handling is performed in a well ventilated place.
2	Wear suitable protective equipment.
3	Avoid contact with skin and eyes.

◆ Measures to prevent fire

1	Keep away from heat/sparks/open flames/ hot surfaces.

◆ Measures to prevent aerosol and dust generation

1	Avoid formation of dust and aerosols.
2	Provide appropriate exhaust ventilation at places where dust is formed.

◆ Advice on general occupational hygiene

1	Wash hands and face after using of the substances.
2	Replace the contaminated clothing immediately.

7.2 Conditions for safe storage, including any incompatibilities

1	Keep containers tightly closed.
2	Keep containers in a dry, cool and well-ventilated place.
3	Keep away from heat/sparks/open flames/hot surfaces.
4	Store away from incompatible materials and foodstuff containers.
5	Store only in the original container in accordance with national regulations (German TRGS 510).
6	Storage class (LGK) according to TRGS 510: 11

7.3 Specific end use(s)

1	In addition to use mentioned in the Section 1.2, unforeseen other specific end uses.

Part 8: Exposure controls/personal protection

8.1 Control parameters

◆Occupational exposure limit values

Occupational Exposure limit values	No relevant regulations

◆Biological limit values

Biological limit values	No relevant regulations

◆Monitoring methods

Monitoring methods	Use suitable workplace exposure monitoring methods in accordance with applicable EU/UK and national requirements. Where applicable, methods meeting EN 482 and EN 14042 may be used. For Germany, monitoring of inhalation exposure should be carried out in accordance with TRGS 402; IFA/DGUV methods may be used where applicable.

◆ Derived No effect level (DNEL)

Component	Route of exposure	DNEL for Workers			
		Acute effects (local)	Acute effects (systemic)	Chronic effects (local)	Chronic effects (systemic)
5,6-Dimethylxantheonone-4-acetic acid	Inhalation	No information available	No information available	No information available	No information available
	Oral	No information available	No information available	No information available	No information available
	Dermal	No information available	No information available	No information available	No information available

◆ Predicted No Effect Concentration (PNEC)

Predicted No Effect Concentration (PNEC)	No information available

8.2 Exposure controls

8.2.1 Engineering controls

1	Ensure adequate ventilation, especially in confined areas.
2	Ensure that eyewash stations and safety showers are close to the workstation location.
3	Set up emergency exit and necessary risk-elimination area.
4	Handle in accordance with good industrial hygiene and safety practice.

8.2.2 Personal protection equipment

General requirement	
Eye protection	Must wear appropriate safety goggles.
Hand protection	Must wear appropriate chemical protective gloves.
Respiratory protection	Must wear appropriate personal respiratory protective equipment.
Skin and body protection	Must wear appropriate chemical protective clothing and chemical resistant shoes.

8.2.3 Environmental exposure controls

Environmental exposure controls	No information available

Part 9: Physical and chemical properties

9.1 Information on basic physical and chemical properties

Physical state	solid
Colour	White to off-white
Odour	No information available
Odour threshold	No information available
pH	No information available
Melting point/freezing point(℃)	No information available
Boiling point or initial boiling point and boiling range(℃)	≥261(101.325 kPa, decomposition at ≥261℃)
Flash point(Closed cup,℃)	Not applicable
Evaporation rate	Not applicable
Flammability	No information available
Lower and upper explosion limit/flammability limit [%(v/v)]	Upper limit: No information available; Lower limit: No information available
Vapour pressure	Not applicable
Relative vapour density(Air = 1)	Not applicable
Relative density(Water=1)	No information available
Solubility(mg/L)	1.35mg/L(19.9 ℃(pH=7.2~7.3))
Partition coefficient n-octanol/water (log value)	No information available
Auto-ignition temperature(℃)	No information available
Decomposition temperature(℃)	No information available
Kinematic viscosity(mm²/s)	Not applicable
Explosive properties	No information available
Oxidizing properties	No information available

Particle characteristics	No information available

9.2 Other information

9.2.1 Information with regard to physical hazard classes

Information with regard to physical hazard classes	No information available

9.2.2 Other safety characteristics

Other safety characteristics	No information available

Part 10: Stability and reactivity

Stability and reactivity

10.1 Reactivity	Contact with incompatible substances can cause decomposition or other chemical reactions.
10.2 Chemical stability	Stable under proper operation and storage conditions.
10.3 Possibility of hazardous reactions	No information available.
10.4 Conditions to avoid	Incompatible materials, heat, flame and spark.
10.5 Incompatible materials	No information available.
10.6 Hazardous decomposition products	Under normal conditions of storage and use, hazardous decomposition products should not be produced.

Part 11: Toxicological information

11.1 Information on hazard classes as defined in Regulation (EC) No 1272/2008 with amendment 2023/707

5,6-Dimethylxantheonone-4-acetic acid(Component)	
Skin corrosion/irritation	Based on available data, the classification criteria are not met
Serious eye damage/irritation	Based on available data, the classification criteria are not met
Skin sensitization	Based on available data, the classification criteria are not met
Respiratory sensitization	Based on available data, the classification criteria are not met
Reproductive toxicity	Based on available data, the classification criteria are not met
STOT-single exposure	Based on available data, the classification criteria are not met
STOT-repeated exposure	Based on available data, the classification criteria are not met
Aspiration hazard	Based on available data, the classification criteria are not met
Germ cell mutagenicity	Based on available data, the classification criteria are not met

Acute toxicity

Acute toxicity	No information available

Carcinogenicity

Component	List of carcinogens by the IARC Monographs	Report on Carcinogens by NTP
5,6-Dimethylxantheonone-4-acetic acid	Not Listed	Not Listed

11.2 Information on other hazards

11.2.1 Human endocrine disrupting properties

Component	Human endocrine disrupting properties
5,6-Dimethylxantheonone-4-acetic acid	No information available

11.2.2 Other Information

Other Information	See Section 11.1

Part 12: Ecological information

12.1 Toxicity

Acute aquatic toxicity

Component	Fish	Crustaceans	Algae or other aquatic plants
5,6-Dimethylxantheonone-4-acetic acid	LC_{50}： > 100mg/L (96h)(Fish)	No information available	No information available

Chronic aquatic toxicity

Chronic aquatic toxicity	No information available

12.2 Persistence and degradability

Persistence and degradability	No information available

12.3 Bioaccumulative potential

Bioaccumulative potential	No information available

12.4 Mobility in soil

Mobility in soil	No information available

12.5 Results of PBT and vPvB assessment

Component	Results of PBT and vPvB assessment [according to (EC) No 1907/2006 with amendment 2020/878]
5,6-Dimethylxantheonone-4-acetic acid	No information available

12.6 Endocrine disrupting properties

Component	Endocrine disrupting properties
5,6-Dimethylxantheonone-4-acetic acid	No information available

12.7 Other adverse effects

	No information available

Part 13: Disposal considerations

13.1 Waste treatment methods

Waste chemicals	Before disposal should refer to the relevant national and local laws and regulation. Recommend the use of incineration disposal.
Contaminated packaging	Containers may still present chemical hazard when empty. Keep away from hot and ignition source of fire. Return to supplier for recycling if possible.

Disposal recommendations	Refer to section waste chemicals and contaminated packaging.

Part 14: Transport information

Label

Transporting Label	

IMDG-CODE

14.1 UN number	3077
14.2 UN proper shipping name	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.
14.3 Transport hazard class	9
14.4 Packing group	Ⅲ
14.5 Environmental hazards (Yes or no)	Yes
14.6 Environmentally Hazardous Substance Mark	
14.7 EmS No.	F-A，S-F

IATA-DGR

14.1 UN number	3077
14.2 UN proper shipping name	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.
14.3 Transport hazard class	9
14.4 Packing group	Ⅲ
14.5 Environmental hazards (Yes or no)	Yes
14.6 Environmentally Hazardous Substance Mark	

UN-ADR

14.1 UN number	3077
14.2 UN proper shipping name	ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S.
14.3 Transport hazard class	9
14.4 Packing group	Ⅲ
14.5 Environmental hazards (Yes or no)	Yes
14.6 Environmentally Hazardous Substance Mark	

Special precautions for user

	Transport vehicles should be equipped with the appropriate variety and quantity of fire equipment and emergency equipment leakage during transport. Before transport, should be preceded by checking whether container integrity, sealing. The transport unit must be placarded and marked in accordance with relevant transporting requirements.

Maritime transport in bulk according to IMO instruments

◆Transport in bulk according to Annex II of MARPOL and the IBC code	
	No information available
◆Transport in bulk in accordance with MARPOL Annex V and the IMSBC Code	
	No information available
◆Transport in bulk in accordance with the IGC Code	
	No information available

Part 15: Regulatory information

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

International chemical inventory

Component	A	B	C	D	E	F	G	H	I	J	K	L	M
5,6-Dimethylxantheonone-4-acetic acid	×	×	×	×	×	×	×	×	×	×	×	√	√

【A】 China Inventory of Existing Chemical Substances(IECSC)
【B】 European Inventory of Existing Commercial Chemical Substances(EC inventory)
【C】 United States Toxic Substances Control Act Inventory(TSCA)
【D】 Canadian Domestic Substances List(DSL)
【E】 New Zealand Inventory of Chemicals(NZIoC)
【F】 Philippines Inventory of Chemicals and Chemical Substances(PICCS)
【G】 Korea Existing Chemicals Inventory(KECL)
【H】 Australian Inventory of Industrial Chemicals(AIIC)
【I】 Japan Inventory of Existing & New Chemical Substances(ENCS)
【J】 Thailand Existing Chemicals Inventory(TECI)
【K】 Mexico National Inventory of Chemical Substances(INSQ)
【L】 Russia Inventory of Existing Substances(DRAFT)
【M】 Inventory of Existing Chemical Substances in Taiwan, China(TCSI)

List of Chemical Substances under International Conventions

Component	A	B	C
5,6-Dimethylxantheonone-4-acetic acid	×	×	×

【A】 The Montreal Protocol on Substances that Deplete the Ozone Layer
【B】 Stockholm Convention on Persistent Organic Pollutants (POPs)
【C】 Rotterdam Convention on the prior informed consent procedure for certain hazardous chemicals and pesticides in international trade

European chemical inventory

Component	A	B	C	D	E	F	G	H
5,6-Dimethylxantheonone-4-acetic acid	×	×	×	√	×	×	×	×

【A】 Candidate list of Substances of Very High Concern for authorisation under EU REACH regulation
【B】 Substances requiring authorisation under EU REACH regulation
【C】 Substances restricted under EU REACH

【D】 Registered substances under EU REACH
【E】 Substance Evaluation – CoRAP under EU REACH
【F】 List of priority substances under EU water policy
【G】 Substances subject to POPs Regulation
【H】 Substances proposed as POPs

Note:
"√" Indicates that the substance included in the regulations.
"×" No data or not included in the regulations.

German water hazard class(WGK)

	WGK 3 – highly hazardous to water (precautionary classification according to AwSV; no published WGK classification available).

German technical instructions on air quality control(TA LUFT)

	No information available

German technical rules for hazardous substances(TRGS)

	No information available

15.2 Chemical safety assessment

	No Chemical Safety Assessment has been carried out for this substance/mixture by the supplier.

Part 16: Other information

Information on revision

Creation Date	2026/10/27
Revision Date	-
Reason for revision	-

Reference

[1] IPCS: The International Chemical Safety Cards (ICSC), website: http://www.ilo.org/dyn/icsc/showcard.home.
[2] IARC, website: http://www.iarc.fr/.
[3] OECD: The Global Portal to Information on Chemical Substances, website: https://www.echemportal.org/echemportal/.
[4] CAMEO Chemicals, website: http://cameochemicals.noaa.gov/search/simple.
[5] NLM: ChemIDplus, website: http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp.
[6] EPA: Integrated Risk Information System, website: http://cfpub.epa.gov/iris/.
[7] U.S. Department of Transportation: ERG, website: http://www.phmsa.dot.gov/hazmat/library/erg.
[8] Germany GESTIS-database on hazard substance, website: http://gestis-en.itrust.de/.

Abbreviations and acronyms

CAS	Chemical Abstracts Service	UN	The United Nations
PC-STEL	Short term exposure limit	OECD	Organisation for Economic Co-operation and Development
PC-TWA	Time Weighted Average	IMDG-CODE	International Maritime Dangerous Goods CODE
MAC	Maximum Allowable Concentration	IARC	International Agency for Research on Cancer
DNEL	Derived No Effect Level	ICAO	International Civil Aviation Organization
PNEC	Predicted No Effect Concentration	IATA	International Air Transport Association
NOEC	No Observed Effect Concentration	ACGIH	American Conference of Governmental Industrial Hygienists
LC_{50}	Lethal Concentration 50%	NFPA	National Fire Protection Association
LD_{50}	Lethal Dose 50%	NTP	National Toxicology Program
EC_{50}	Effective Concentration 50%	PBT	Persistent, Bioaccumulative, Toxic
EC_X	Effective Concentration X%	vPvB	very Persistent, very Bioaccumulative
P_{OW}	Partition coefficient Octanol: Water	CMR	Carcinogens, mutagens or substances toxic to reproduction
BCF	Bioconcentration factor	RPE	Respiratory Protective Equipment
ED	Endocrine disruptor	G1	Carcinogenic to humans
G2A	Probably carcinogenic to humans	G2B	Possibly carcinogenic to humans

G3	Not yet classified as carcinogenic to humans	G4	Probably not carcinogenic to humans

Disclaimer

This Safety Data Sheet (SDS) was prepared according to REACH Regulation The data included was derived from international authoritative database and provided by the enterprise. Other information was based on the present state of our knowledge. We try to ensure the correctness of all information. However, due to the diversity of information sources and the limitations of our knowledge, this document is only for user's reference. Users should make their independent judgment of suitability of this information for their particular purposes. We do not assume responsibility for loss, damage or expense arising out of or in any way connected with the handling, storage, use or disposal of the product.